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VOLUME 9

Standard X-ray Diffraction Powder Patterns



UNITED STATES DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

THE NATIONAL BUREAU OF STANDARDS

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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Marlene I. Cook, Thelma Isaacs, and Eloise H. Evans



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Contents

	Page		Page
Introduction-----	1	Holmium sesquioxide, Ho_2O_3 -----	32
Standard X-ray powder patterns:		Magnesium chromite (picrochromite), MgCr_2O_4 ---	34
Aluminum oxide-alpha (corundum), $\alpha\text{-Al}_2\text{O}_3$ -----	3	Manganese aluminate (galaxite), MnAl_2O_4 -----	35
Ammonium azide, NH_4N_3 -----	4	Manganese ferrite (jacobsite), MnFe_2O_4 -----	36
Ammonium bicarbonate (teschemacherite), $(\text{NH}_4)\text{HCO}_3$ -----	5	Manganese(III) oxide (partridgeite), Mn_2O_3 ----	37
Ammonium bromoplatinate, $(\text{NH}_4)_2\text{PtBr}_6$ -----	6	Mercury(II) oxide (montroydite), HgO -----	39
Ammonium perrhenate, NH_4ReO_4 -----	7	Neodymium ethylsulfate nonahydrate, $\text{Nd}[(\text{C}_2\text{H}_5)_2\text{SO}_4]_3 \cdot 9\text{H}_2\text{O}$ -----	41
Ammonium sulfate (mascagnite), $(\text{NH}_4)_2\text{SO}_4$ -----	8	Nickel aluminate, NiAl_2O_4 -----	42
Beryllium aluminum oxide (chrysoberyl), BeAl_2O_4	10	Nickel germanate, Ni_2GeO_4 -----	43
Beryllium aluminum silicate (beryl), $\text{Be}_3\text{Al}_2(\text{SiO}_3)_6$	13	Potassium borohydride, KBH_4 -----	44
Bismuth oxyiodide, BiOI -----	16	Potassium cobaltinitrite, $\text{K}_3\text{Co}(\text{NO}_2)_6$ -----	45
Cadmium bromide, CdBr_2 -----	17	Potassium heptafluorozirconate, K_3ZrF_7 -----	46
Cadmium chloride, CdCl_2 -----	18	Praseodymium oxychloride, PrOCl -----	47
Calcium aluminate 12:7, $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$ -----	20	Silver iodide, gamma, $\gamma\text{-AgI}$ -----	48
Calcium iron silicate (andradite), $\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$ ---	22	Silver metaperiodate, AgIO_4 -----	49
Cesium bromotellurate, Cs_2TeBr_6 -----	24	Sodium borohydride, NaBH_4 -----	51
Cesium nitrate, CsNO_3 -----	25	Strontium zirconate, SrZrO_3 -----	51
Chromium orthophosphate beta, $\beta\text{-CrPO}_4$ -----	26	Sulfur, S-----	54
Cobalt aluminum oxide, CoAl_2O_4 -----	27	Tellurium(IV) oxide (tellurite), TeO_2 -----	57
Cobalt(II) oxide, CoO -----	28	Thulium sesquioxide, Tm_2O_3 -----	58
Cobalt(II, III) oxide, Co_3O_4 -----	29	Titanium(III) oxide, $\text{TiO}_{1.515}$ -----	59
Dysprosium sesquioxide, Dy_2O_3 -----	30	Zinc iodide, ZnI_2 -----	60
Erbium phosphate, ErPO_4 -----	31	Cumulative index to volumes 1, 2, 3, 4, 5, 6, 7, 8, and 9	62

Errata

Vol. 5. Page 5, calculated density for ammonium chlorostannate should be 2.398 g/cm³.

Vol. 6. Page 15, the *d*-values of the NBS pattern should read 1.4361 instead of 1.4351 and 1.3184 instead of 1.3148.

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. 9—Data for 43 Substances

Howard E. Swanson, Marlene I. Cook,¹ Thelma Isaacs,¹ and Eloise H. Evans¹

Forty-three standard X-ray diffraction powder patterns are presented. Thirty-one are to replace forty-one patterns already given in the X-ray Powder Data File, and twelve are for substances not previously included. The X-ray Powder Data File is a compilation of diffraction patterns from all sources and is used for the identification of unknown crystalline materials by matching spacing and intensity measurements. In this Circular, comparison is made of all powder diffraction data available for each of the substances reported. The patterns were made with a Geiger counter X-ray diffractometer, using samples of high purity. The d -values were assigned Miller indices determined by comparison with calculated interplanar spacings and from space group considerations. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible.

Included are X-ray data for the following forty-three substances: α - Al_2O_3 (corundum), NH_4N_3 , $(\text{NH}_4)\text{HCO}_3$ (teschemacherite), $(\text{NH}_4)_2\text{PtBr}_6$, NH_4ReO_4 , $(\text{NH}_4)_2\text{SO}_4$ (mascagnite), BeAl_2O_4 (chrysoberyl), $\text{Be}_3\text{Al}_2(\text{SiO}_3)_6$ (beryl), BiOI , CdBr_2 , CdCl_2 , $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$, $\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$ (andradite), Cs_2TeBr_6 , CsNO_3 , β - CrPO_4 , CoAl_2O_4 , CoO , Co_3O_4 , Dy_2O_3 , ErPO_4 , Ho_2O_3 , MgCr_2O_4 (picrochromite), MnAl_2O_4 (galaxite), MnFe_2O_4 (jacobsonite), Mn_2O_3 (partridgeite), HgO (montroydite), $\text{Nd}[(\text{C}_2\text{H}_5)\text{SO}_4]_3 \cdot 9\text{H}_2\text{O}$, NiAl_2O_4 , Ni_2GeO_4 , KBH_4 , $\text{K}_3\text{Co}(\text{NO}_2)_6$, K_3ZrF_7 , PrOCl , γ - AgI , AgIO_4 , NaBH_4 , SrZrO_4 , S , TeO_2 (tellurite), Tm_2O_3 , $\text{TiO}_{1.615}$, and ZnI_2 .

INTRODUCTION

The National Bureau of Standards in its program² for the revision and evaluation of published X-ray data for the X-ray Powder Data File presents data for 43 compounds. This paper is the ninth of a series of "Standard X-ray Diffraction Powder Patterns". These patterns are recommended to replace 41 cards now in the file. The patterns for 12 compounds not represented in the file have been added. These compounds are ammonium bromoplatinate, ammonium perhenate, cadmium bromide, cesium bromotellurate, dysprosium sesquioxide, erbium phosphate, holmium sesquioxide, neodymium ethylsulfate nonahydrate, nickel germanate, potassium cobaltinitrite, preaseodymium oxychloride, and sodium borohydride.

The experimental procedure and general plan of these reports have not changed from that of the previous volumes of the NBS Circular.³ However, the basic technique is discussed, in this section, under the same headings that appear in the text of this volume.

ASTM cards. Each section of this Circular contains a table listing the ASTM file card numbers, the three strongest lines, the radiations used, and the literature references for each card. Cards listed in the 1958 index to the Powder Data File [1]⁴ are included in the table.

Additional published patterns. Literature references and radiation data for patterns that have not been published as ASTM cards are listed. These patterns are included in the tables of d -values and intensities.

NBS sample. Many of the samples used to make NBS patterns were special preparations (of exceptionally high purity) obtained or prepared only in small quantities. Unless otherwise noted, the spectrographic analysis was done at NBS after recrystallization or heat treatment. The limit of detection for the alkali elements is 0.05 percent for the spectrographic analysis. A phase-purity check was made on the nonopaque materials during the refractive index determination. Another check of phase-purity was provided by the X-ray pattern itself, since it was indexed by comparison with theoretical d -values. Treating the sample by appropriate annealing, recrystallizing, or heating in hydrothermal bombs improved the quality of most of the patterns.

At least two intensity patterns were prepared to check reproducibility of measured values. Samples that gave satisfactory intensity patterns usually had a particle-size average well within the range of 5 to 10 μ , as suggested by Alexander, Klug, and Kummer [2]. A special cell with one open end was used for making intensity measurements. An intensity sample was prepared by clamping a flat piece of glass temporarily over the surface of this holder, and while it was held in a vertical position, the sample was drifted in from the open end. The glass was then carefully removed so that the surface of the sample could be exposed to the X-ray beam. For a few powder samples that did not flow readily or were prone to orient excessively, approximately 50-volume percent of finely ground silica-gel was added

¹ Fellow at the National Bureau of Standards sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods.

² This project is sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods. This committee is composed of members from the American Society for Testing Materials, the American Crystallographic Association, and the British Institute of Physics. Financial support is also provided by the National Bureau of Standards.

³ Other volumes were published as follows: Vol. 1 and Vol. 2 June 1953; Vol. 3, June 1954; Vol. 4, March 1955; Vol. 5, October 1955; Vol. 6, September 1956; Vol. 7, September 1957; and Vol. 8, April 1959.

⁴ Figures in brackets indicate the literature references at the end of each section of this paper.

as a diluent. The intensity values of each pattern were measured as peak height above background and are expressed as percentages of the strongest line. Additional patterns were obtained for d -value measurements. These specimens were prepared by packing into a shallow holder a sample containing approximately 5-weight percent of tungsten powder that served as an internal standard. The lattice constant used for tungsten at 25°C is 3.1648 Å, as determined by Jette and Foote [3]. All of the NBS patterns, unless otherwise noted, are made at 25°C, using either filtered copper radiation ($K\alpha_1$), cobalt radiation ($K\alpha_1$), or iron radiation ($K\alpha_1$), having the wavelengths 1.5405 Å, 1.7889 Å, and 1.9360 Å, respectively.

Interplanar spacings and intensity measurements.

Interplanar spacing data presented in the tables were converted to angstrom units as internationally defined in 1946 [4]. The conversions were from Bragg angle data, from d -values in kX units using the factor 1.00202, or from d -values based on wavelengths given in other than kX units. In each case, the type of conversion is indicated. The wavelength values in the tables of d -values and intensities are given in angstrom units, whereas the wavelengths listed under the first section of each report are the original values taken from the literature. The tables of patterns contain data based on the original work rather than that data reported on the ASTM cards if there is a difference.

Abbreviations used when describing intensities, taken from the literature, without numerical values are: s, strong; m, medium; and w, weak. Other abbreviations used are: B, broad; D, diffuse; db, doublet; and v, very.

Structural data. Although the NBS lattice constants of cubic materials were calculated for each d -value, the constant reported is that obtained by averaging the last five lines because of the greater accuracy of measurement in the large-angle region of the pattern. The unit-cell values for each non-cubic substance were determined by means of a least-squares calculation made by the IBM 704 from the latter half of the pattern, using those d -values for which there was only one possible Miller Index. The number of significant figures reported in the NBS pattern is limited by the quality of each sample and by its structural symmetry.

Published unit-cell data were converted to angstrom units in the same manner as were the published d -values. When cell values based upon more than one cell configuration have been taken from the literature, corrections that were made to make them comparable have been indicated. The limits of error generally published with unit-cell data have not been included in the table because the number of determinations and their accuracy and variations were such that a statistical evaluation would be unjustified.

Starting with volume 8 we have adopted a variation in our routine for presenting the space group. In place of both the Schoenflies symbol and the International symbol previously listed, we have dropped the Schoenflies symbol and added the space group number in the International Tables for X-ray Crystallography. It is felt that this number has become useful in locating space group data, while the use of the Schoenflies symbol has diminished.

We have also decided to present orthorhombic cell dimensions only in the "standard" arrangement of a , b , c , as given in the International Tables rather than with a permutation as is occasionally given in the literature.

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are based upon atomic weights reported by E. Wichers [5] in 1956 and the Avogadro number (6.0240×10^{23}) reported by Straumanis [6] in 1954. The refractive index measurements were made by grain-immersion methods in white light using oils standardized in sodium light.

References

- [1] Index to the X-ray powder data file, American Society for Testing Materials, Philadelphia, Pa. (1958).
- [2] L. Alexander, H. P. Klug, and E. Kummer, Statistical factors affecting the intensity of X-rays diffracted by crystalline powders, *J. Appl. Phys.* **19**, No. 8, 742-753 (1948).
- [3] E. R. Jette and F. Foote, Precision determination of lattice constants, *J. Chem. Phys.* **3**, 605-616 (1935).
- [4] Anonymous, The conversion factor for kX units to angstrom units, *J. Sci. Inst.* **24**, 27 (1947).
- [5] E. Wichers, Report of the Committee on Atomic Weights of the American Chemical Society. *J. Am. Chem. Soc.* **78**, 3235 (1956).
- [6] M. E. Straumanis, Remark concerning the absolute value of Avogadro's number, *Phys. Rev.* **95**, 566 (1954).

alpha-Aluminum Oxide (corundum), α -Al₂O₃ (trigonal)

ASTM cards

The following pattern is the same pattern shown on ASTM card 5-0712 [1] prepared in 1953 by NBS, but thirteen additional lines have been included. These weak lines were brought out by slower scanning.

NBS sample. The same Mallinckrodt sample was used. It was annealed at 1,400°C for 4 hr in an Al₂O₃ crucible.

Structural data. Bragg [2] in 1922 determined that alpha-aluminum oxide has the corundum-type structure, the space group R $\bar{3}c$ (No. 167) with 6(Al₂O₃) per unit hexagonal cell or 2(Al₂O₃) per unit rhombohedral cell.

Lattice constants

		<i>a</i>	<i>c</i>
		<i>A</i>	<i>A</i>
1953	National Bureau of Standards-----	4.758	12.991 at 26° C

The density of alpha-aluminum oxide calculated from NBS lattice constants is 3.987 g/cm³ at 26° C.

References

- [1] NBS (U.S.) Circ. 539 2, 20-23 (1953).
- [2] W. H. Bragg, The significance of crystal structure, J. Chem. Soc. London 121, 2766-2787 (1922).

<i>hkl</i> hex.	1959	
	National Bureau of Standards	
	Cu, 1.5405 Å at 26° C	
	<i>d</i>	<i>I</i>
	<i>A</i>	
012	3.479	74
104	2.552	92
110	2.379	42
006	2.165	<1
113	2.085	100
202	1.964	1
024	1.740	43
116	1.601	81
211	1.546	3
122	1.514	4
018	1.510	7
124	1.404	32
030	1.374	48
125	1.337	1
208	1.276	2
1·0·10	1.239	16
119	1.2343	7
220	1.1898	6
306	1.1600	<1
223	1.1470	4
311	1.1382	1
312	1.1255	5
128	1.1246	2
0·2·10	1.0988	6
0·0·12	1.0831	3
134	1.0781	7
226	1.0426	13
402	1.0175	1
1·2·10	0.9976	11
1·1·12	.9857	<1
404	.9819	2
321	.9431	<1
1·2·11	.9413	<1
318	.9345	3
229	.9178	2
324	.9076	12
0·1·14	.9052	3
410	.8991	6
235	.8884	<1
413	.8804	4
048	.8698	2
1·3·10	.8580	12
3·0·12	.8502	4
2·0·14	.8460	4
146	.8303	22
1·1·15	.8137	4
4·0·10	.8072	11
054	.7988	7
1·0·16	.7970	14
330	.7931	13

Ammonium Azide, NH_4N_3 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
3-0687	2.89 3.12 3.83	Molybdenum	Dow Chemical Co., Midland, Michigan.

Additional published patterns

Source	Radiation
Frevel [1] 1936.....	Copper K_α

NBS sample. The sample of ammonium azide was prepared in Prof. F. O. Rice's laboratory at the Catholic University of America by E. Miller by neutralizing hydrazoic acid in ether solution with ammonia and crystallizing. The sample was dried over calcium chloride.

The sample is colorless and optically negative. The indices of refraction are $N_\alpha = 1.511$, $N_\beta = 1.606$, $N_\gamma = 1.688$, and $2V = 88^\circ$.

Interplanar spacings and intensity measurements. The d -values reported by the Dow Chemical Co. and by Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Dow Chemical Co.	210, 012	202	010
Frevel	202	010	103, 211
National Bureau of Standards	210	012	202

Structural data. Frevel [1] in 1936 determined that ammonium azide has the ammonium hydrofluoride-type structure, the space group Pnma (No. 53), and $4(\text{NH}_4\text{N}_3)$ per unit cell.

The unit-cell measurements reported by Frevel have been converted from kX to angstrom units for comparison with NBS values.

hkl	Dow Chemical Co.		1936 Frevel		1959 National Bureau of Standards	
	Mo, 0.7107 Å		Cu, 1.5418 Å		Cu, 1.5405 Å at 25°C	
	d	I	d	I	d	I
	A		A		A	I
200	-----	---	4.48	15	4.48	10
002	-----	---	4.32	18	4.33	11
010	3.84	40	3.81	50	3.811	39
202	3.13	60	3.11	100	3.111	70
210	} 2.90	100	-----	---	2.899	100
012					2.860	100
301	-----	---	-----	---	2.820	35
103	} 2.77	40	2.75	35	2.748	42
211					-----	---
112	-----	---	-----	---	2.723	6
013	-----	---	-----	---	2.302	5
311	-----	---	2.266	25	2.265	18
400	} 2.23	20	2.227	30	2.232	22
113					2.229	20
004	2.18	10	2.163	15	2.166	9
312	-----	---	2.056	5	2.063	3
402	-----	---	-----	---	1.986	2
204	-----	---	1.947	10	1.950	3
020	1.91	10	1.903	18	1.904	9
021	-----	---	1.860	5	1.860	2
313	} -----	---	-----	---	1.822	1
121					-----	---
412	-----	---	1.757	8	1.760	7
220	} -----	---	-----	---	1.751	7
501					-----	---
214	-----	---	1.736	10	1.735	2
122	-----	---	-----	---	1.711	3
105	-----	---	1.702	10	1.702	2
222	-----	---	-----	---	1.623	6
413	-----	---	-----	---	1.602	---
511, 314	} -----	---	1.589	5	1.591	3
023					-----	---
321	-----	---	-----	---	1.579	1
123	-----	---	-----	---	1.565	2
404	} -----	---	1.554	5	1.553	2
115					-----	---
512	-----	---	-----	---	1.515	1
322	-----	---	-----	---	1.503	2
305	} -----	---	-----	---	1.4981	5
223					-----	---
414	-----	---	-----	---	1.4399	3
421	} -----	---	1.430	10	1.4294	5
024					-----	---
513	} -----	---	-----	---	1.4116	2
124					-----	---
602	-----	---	-----	---	1.4087	4
610	-----	---	1.388	5	1.3866	3
422	} -----	---	1.374	5	1.3742	2
206					-----	---
611	-----	---	-----	---	1.3700	1
016	-----	---	1.350 (*)	5	1.3501	2

* Six additional lines were omitted.

The density of ammonium azide calculated from NBS lattice constants is 1.353 g/cm³ at 25° C.

		<i>a</i>	<i>b</i>	<i>c</i>
1936	Frevel [1]-----	<i>A</i> 8.948	<i>A</i> 3.808	<i>A</i> 8.659
1959	National Bureau of Standards-----	8.936	3.809	8.663 at 25° C

References

[1] L. K. Frevel, The crystal structure of ammonium azide, NH₄N₃, Z. Krist. 94A, 197-211 (1936).

Ammonium Bicarbonate, (teschemacherite), (NH₄)HCO₃ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0868	2.99 5.3 4.02	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of ammonium bicarbonate was obtained from Baker and Adamson Chemical Co., New York. Spectrographic analysis detected no impurities.

The sample is colorless and optically negative. The refractive indices are $N_\alpha = 1.421$, $N_\beta = 1.535$, $N_\gamma = 1.554$. $2V = 24^\circ$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and

<i>hkl</i>	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 Å		1959 National Bureau of Standards Cu, 1.5405 Å at 25° C		<i>hkl</i>	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 Å		1959 National Bureau of Standards Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>		<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	<i>A</i>		<i>A</i>						
110	-----	-----	5.98	4	313	-----	-----	1.8342	2
020	5.3	42	5.34	59	400	-----	-----	1.8137	4
002	-----	-----	4.39	4	060	-----	-----	1.7843	3
012	4.03	27	4.05	45	341	}-----	-----	1.7564	2
102	-----	-----	3.74	10	323				
200	3.62	27	3.62	57	411	-----	-----	1.7514	3
022	3.40	7	3.39	12	252	}-----	3	1.6995	4
211	3.20	7	3.195	18	153			1.6794	3
122	3.07	10	3.068	30	115			1.6502	3
131	} 3.00	100	3.005	43	333			1.6207	5
220			2.998	100	125	-----	-----	1.6019	2
221	-----	-----	2.841	6	260	-----	-----	1.5898	3
202	2.80	3	2.794	12	431	-----	-----	1.5757	<1
212	2.70	7	2.701	18	261	-----	-----	1.5515	2
113	2.62	7	2.624	21	324	-----	-----	1.5345	<1
222	-----	-----	2.476	7	244	-----	-----	1.5165	1
231	-----	-----	2.443	17	432	-----	-----	1.5021	1
141	} 2.42	10	2.413	8	440	-----	-----	1.4752	2
123					171	-----	-----	1.4349	3
042	} 2.28	3	2.282	4	145	-----	-----	1.4180	<1
311					511	-----	-----	1.4044	2
142	-----	-----	2.1781	20	353	}-----	-----	1.3846	2
240	2.15	20	2.1547	29	315				
302	-----	-----	2.1152	11	263				
104	2.09	3	2.0938	6	414	-----	-----	1.3639	1
024	-----	-----	2.0238	4	362	-----	-----		
151	-----	-----	1.9993	4					
331	}-----	-----	1.9505	2					
124									
204			1.8721	2					

Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel - National Bureau of Standards -	131, 220 220	020 020	012 200

Structural data. Mooney [2] in 1932 determined that ammonium bicarbonate has the space group P_{63} (No. 56), with $8[(\text{NH}_4)\text{HCO}_3]$ per unit cell.

The unit-cell measurements reported by Mooney have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		<i>A</i>	<i>A</i>	<i>A</i>
1932	Mooney [2]-----	7.30	10.81	8.78
1959	National Bureau of Standards-----	7.255	10.709	8.746 at 25° C

The density of ammonium bicarbonate calculated from the NBS lattice constants is 1.545 g/cm³ at 25° C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem. Anal. Ed. 10, 457-512 (1938).
- [2] R. C. L. Mooney, Crystal structure of ammonium bicarbonate, Phys. Rev. 39, 861-862 (1932).

Ammonium Bromoplatinate, $(\text{NH}_4)_2\text{PtBr}_6$ (cubic)

<i>hkl</i>	1959 National Bureau of Standards Cu, 1.5405 Å at 25° C			<i>hkl</i>	1959 National Bureau of Standards Co, 1.7889 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>		<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>				
111	5.99	94	10.38	844	1.0584	8	10.370
200	5.18	100	10.38	933	1.0421	3	10.369
220	3.664	6	10.36	10·0·0	1.0369	3	10.369
311	3.127	48	10.37	10·2·0	1.0166	1	10.367
222	2.994	53	10.37	951	1.0024	5	10.369
400	2.592	90	10.369	10·2·2	0.9977	<1	10.368
331	2.378	14	10.368	953	.9669	4	10.369
420	2.3189	60	10.370	10·4·0	.9627	4	10.369
422	2.1166	3	10.369	10·4·2	.9466	1	10.369
511	1.9954	28	10.368	11·1·1	.9348	<1	10.367
440	1.8329	52	10.368	880	.9164	1	10.368
531	1.7524	25	10.367	11·3·1	.9058	1	10.367
600	1.7281	27	10.369	10·4·4	.9024	3	10.368
620	1.6394	2	10.368	10·6·0	.8890	2	10.367
533	1.5813	6	10.369	11·3·3	.8793	<1	10.367
622	1.5634	9	10.370	10·6·2	.8761	1	10.366
444	1.4966	17	10.369	12·0·0	.8639	2	10.367
711	1.4519	13	10.369	11·5·1	.8551	1	10.367
640	1.4381	11	10.370	12·2·0	.8522	2	10.367
642	1.3858	2	10.370	12·2·2	.8409	1	10.367
731	1.3501	7	10.370	11·5·3	.8327	2	10.367
800	1.2960	5	10.368	12·4·0	.8196	2	10.367
820	1.2573	9	10.368	991	.8120	2	10.367
822	1.2220	1	10.369	12·4·2	.8095	3	10.367
751	1.1973	4	10.369	10·8·2	.7998	1	10.367
662	1.1893	2	10.368	13·1·1	.7927	3	10.366
840	1.1592	12	10.368	Average value of last five lines---			10.367
911	1.1382	5	10.369				
842	1.1314	6	10.369				
931	1.0869	3	10.368				

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium bromoplatinate was prepared at NBS from bromoplatinic acid and ammonium bromide. Spectrographic analysis showed no impurities greater than 0.001 percent.

The color of the sample was deep orange. The index of refraction was too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The indices of the three strongest lines of NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards-----	200	111	400

Ammonium Perrhenate, NH_4ReO_4 (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium perrhenate was obtained from the Johnson, Matthey and Co., London, England. Their spectrographic analysis detected calcium and magnesium (very faintly visible) as the only impurities.

The sample is colorless and optically positive. The refractive indices are $N_o = 1.646$ and $N_e = 1.679$.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards-----	112	101	211

Structural data. Beintema [1] in 1937 determined that ammonium perrhenate has calcium tungstate-type structure, the space group $I4_1/a$ (No. 88) and $4(\text{NH}_4\text{ReO}_4)$ per unit cell.

The unit-cell measurements reported by Beintema have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>a</i>	<i>c</i>
		$\text{\AA}$	$\text{\AA}$
1937	Beintema [1]-----	5.883	12.968
1959	National Bureau of Standards-----	5.883	12.979 at 25° C

Structural data. No structural data for ammonium bromoplatinate was found. Due to the similarity of patterns, it is believed to be isostructural with potassium chloroplatinate, with space group $Fm3m$ (No. 225) and $4[(\text{NH}_4)_2\text{PtBr}_6]$ per unit cell.

Lattice constants

		<i>A</i> 25° C
1959	National Bureau of Standards-----	10.367 at 25° C

The density of ammonium bromoplatinate calculated from NBS lattice constant is 4.235 g/cm^3 at 25° C.

<i>hkl</i>	1959 National Bureau of Standards Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>
	$\text{\AA}$	
101	5.361	71
112	3.504	100
004	3.245	13
200	2.942	18
202	2.680	2
211	2.581	20
114	2.560	3
105	2.3749	8
213	2.2477	12
204	2.1791	19
220	2.0800	8
222	1.9803	1
301	1.9391	5
116	1.9193	11
215	1.8479	11
312	1.7885	19
107	1.7685	4
224	1.7511	9
321	1.6189	6
305	1.5647	3
323	1.5267	6
217	1.5156	5
400	1.4706	2
411	1.4182	7
316	1.4108	8
109	1.4009	3
325	1.3817	2
332	1.3558	5
307	1.3472	3
404	1.3397	3
420	1.3155	4
228	1.2793	1
219	1.2647	1
415	1.2504	1
1·1·10	1.2390	2

Ammonium Perrhenate, NH_4ReO_4 (tetragonal)

The density of ammonium perrhenate calculated from the NBS lattice constants is 3.965 g/cm^3 at 25°C .

<i>hkl</i>	1959 National Bureau of Standards Cu, 1.5405 Å at 25°C	
	<i>d</i>	<i>I</i>
327	1.2251	1
424	1.2192	2
501	1.1717	2
336	1.1677	1
309	1.1615	<1
1·0·11	1.1570	<1
512	}	3
503		
417		
408		
514	1.0866	1
329	1.0805	1
2·1·11	1.0767	1
505	1.0714	1
3·1·10	1.0643	1
523	1.0592	<1
440	1.0397	<1
516	1.0183	2
2·0·12	1.0150	2
525	1.0070	<1
532	0.9971	1
507	.9931	<1
444	.9907	1

References

- [1] J. Beintema, Die Kristallstruktur der Alkaliperperrhenate und-perjodate, Z. Krist. **97A**, 300-322 (1937).

Ammonium Sulfate (mascagnite), $(\text{NH}_4)_2\text{SO}_4$ (orthorhombic)

ASTM cards

$4[(\text{NH}_4)_2\text{SO}_4]$ per unit cell [2]. Unit-cell values were obtained using both old and new spacings for angles higher than $40^\circ (2\theta)$.

Card number	Index lines	Radiation	Source
7-2	4.33 4.39 3.06	Copper	National Bureau of Standards [1] 1956.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		<i>A</i>	<i>A</i>	<i>A</i>
1956	National Bureau of Standards-----	7.782	5.994	10.64 at 25°C
1959	National Bureau of Standards-----	7.782	5.993	10.636 at 25°C

Some time ago Dr. deWolff pointed out that the above pattern did not include some additional weak lines that he had measured.

In order to make the above card more complete we have rerun the Johnson Matthey sample used previously. Fine crystals were prepared by adding alcohol to a water solution of the salt. Slow scanning produced the following expanded pattern.

Interplanar spacings and intensity measurements. The original spacings and intensities remain almost unchanged but 28 new lines have been added.

Structural data. Indexing of the powder pattern is based upon the space group Pnma (No. 62) with

The calculated density is 1.769 g/cm^3 at 25°C .

References

- [1] National Bureau of Standards (U.S.), Circ. 539 **6**, 12 (1956).
[2] A. Ogg, The crystal structure of the isomorphous sulfates of potassium, ammonium, rubidium, and cesium, Phil. Mag. **5**, 354-367 (1928).

Ammonium Sulfate (mascagnite), (NH₄)₂SO₄ (orthorhombic)

hkl	1959		hkl	1959	
	National Bureau of Standards			National Bureau of Standards	
	Cu, 1.5405 Å at 25° C			Cu, 1.5405 Å at 25° C	
	d	I		d	I
	A				
002	5.31	14	033	1.7400	<1
011	5.22	27	106	1.7275	1
102	4.39	63	133	1.6989	2
111	4.33	100			
200	3.890	35	116	1.6609	<1
			413	1.6401	4
201	3.660	<1	420	1.6324	4
210	3.264	<1	206	} 1.6130	2
103	3.227	1	421		
202	3.139	30			
211	3.122	22	233	1.5878	<1
			324	1.5788	<1
013	3.055	54	134	1.5647	1
020	2.998	23	422	1.5603	<1
113	2.839	1	026	1.5244	4
212	2.782	3			
121	2.704	5	040	} 1.4973	5
			126		
004	2.655	13	502		
022	2.611	6	234	1.4938	5
301	2.521	9	017	1.4782	1
122	2.476	2		1.4734	3
213	2.401	3	171	} 1.4467	<1
			333		
220	2.374	2	405		
311	2.322	17	503	} 1.4236	3
221	2.317	18	316		
123	} 2.196	8			
204				226	1.4207
			240	1.3985	1
222	2.168	14	712	1.3774	<1
303	2.093	4	432	1.3473	<1
214	2.062	<1	522	1.3369	2
015	2.005	<1			
223	1.973	4	514	} 1.3109	<1
			406		
400	1.945	4	044		
115	1.942	5	433	} 1.2973	2
321	} 1.927	<1	600		
124					
401			1.914	3	144, 601
			523		
131	1.904	1	317	1.2806	<1
205	1.867	1	118	} 1.2598	<1
304	1.8557	<1	602		
402	1.8270	<1			
132	1.8178	<1	515	1.2298	1
			531	1.2200	1
230	1.7762	1	426	1.2008	1
006	1.7729	3			

Beryllium Aluminum Oxide (chrysoberyl), BeAl_2O_4 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
2-1226	2.08 1.61 3.24	Copper	British Museum.

Additional published patterns

Source	Radiation
Gjessing, Larsson, and Major [2] 1942.... Foster and Royal [3] 1949..... Budnikov, Avetikov, Dudavskij, and Zvjagilskij [4] 1949.....	Iron Copper Chromium

NBS sample. The sample of chrysoberyl was prepared by E. N. Bunting at NBS by heating beryllium oxide and aluminum oxide at $1,300^\circ\text{C}$ and reheating, after grinding, to $1,400^\circ\text{C}$. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of chromium, iron, sodium, and silicon; 0.001 to 0.01 percent each of calcium, magnesium, manganese, and vanadium.

The sample is colorless. The indices of refraction could not be determined because the particle size was too fine.

Interplanar spacings and intensity measurements. The d -values reported by Budnikov, Avetikov, Dudavskij, and Zvjagilskij were converted from kX to angstrom units. The d -values reported by Gjessing, Larsson, and Major were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
British Museum.....	221	222	111
Gjessing, Larsson, and Major.....	221	222	620
Foster and Royal.....	221	222	111
Budnikov, Avetikov, Dudavskij, and Zvjagilskij.....	222	620	040
National Bureau of Standards.....	221	222	111

Structural data.. Bragg and Brown [1] in 1926 determined that chrysoberyl has the space group $Pnma$ (No. 62) and 4(BeAl_2O_4) per unit cell. Their unit-cell measurements have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	b	c
1926	Bragg and Brown [1].....	A	A	A
		9.409	5.481	4.429
1959	National Bureau of Standards.....	9.4041	5.4756	4.4267 at 25°C

The density of chrysoberyl calculated from NBS lattice constants is 3.699 g/cm^3 at 25°C .

References

- [1] W. L. Bragg and G. B. Brown, The crystal structure of chrysoberyl, *Z. Krist.* **63**, 122 (1926).
- [2] L. Gjessing, T. Larsson, and H. Major, Isomorphous substitutes for aluminum in the compound Al_2BeO_4 , *Norsk. Geol. Tidsskr.* **22**, 92-99 (1942).
- [3] W. R. Foster and H. F. Royal, An intermediate compound in the system $\text{BeO} \cdot \text{Al}_2\text{O}_3$ - Al_2O_3 , *J. Am. Ceram. Soc.* **32**, 26-34 (1949).
- [4] P. P. Budnikov, V. G. Avetikov, E. P. Dudavskij, and A. A. Zvjagilskij, The compound $\text{BeO} \cdot 3\text{Al}_2\text{O}_3$, *Doklady Akad. Nauk. SSSR* **68**, 313-316 (1949).

hkl	----- British Museum Cu, 1.541 A		1942 Gjessing, Larsson and Major Fe, 1.936 A		1949 Foster and Royal Cu, 1.5405 A		1949 Budnikov, Avetikov, Dudavskij and Zvjagilskij Cr, 2.2909 A		1959 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A	
200	----- 4.47 -----	----- 40 -----	----- 4.00 -----	----- 12 -----	----- 3.99 -----	----- 30 -----	----- ----- -----	----- ----- -----	----- 4.71 -----	----- 6 -----
101	4.03	60	4.00	12	3.99	30	-----	-----	4.01	49
210	3.60	50	3.56	12	-----	-----	-----	-----	3.570	4
011	-----	-----	-----	-----	-----	-----	-----	-----	3.441	4
111	3.24	80	3.24	50	3.22	50	3.29	20	3.232	86
-----	2.85	40	-----	-----	-----	-----	3.03	10	-----	-----
211	-----	-----	-----	-----	-----	-----	2.84	15	2.777	4
020	-----	-----	-----	-----	-----	-----	-----	-----	2.737	3
301	2.57	80	2.56	50	2.54	50	2.57	25	2.559	52

Beryllium Aluminum Oxide (chrysoberyl), BeAl₂O₄ (orthorhombic)

<i>hkl</i>	----- British Museum		1942 Gjessing, Larsson and Major		1949 Foster and Royal		1949 Budnikov, Avetikov, Dudavskij and Zvjagilskij		1959 National Bureau of Standards	
	Cu, 1.541 Å		Fe, 1.936 Å		Cu, 1.5405 Å		Cr, 2.2909 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
220	-----	-----	2.37	0	-----	-----	-----	-----	2.366	7
311	2.33	80	2.31	50	2.31	30	2.30	20	2.317	30
121	2.26	70	2.26	50	2.25	50	2.25	30	2.260	42
002	-----	-----	-----	-----	-----	-----	-----	-----	2.212	<1
410	-----	-----	-----	-----	-----	-----	-----	-----	2.159	6
102	-----	-----	-----	-----	-----	-----	-----	-----	2.155	3
221	2.08	100	2.08	100	2.08	100	2.07	50	2.087	100
401	-----	-----	-----	-----	-----	-----	-----	-----	2.078	58
112	1.98	20	2.00	0	-----	-----	1.99	<10	2.006	4
411	-----	-----	-----	-----	-----	-----	-----	-----	1.941	2
212	1.88	20	-----	-----	-----	-----	-----	-----	1.880	3
321	-----	-----	1.87	6	-----	-----	1.86	10	1.870	6
302	1.80	60	-----	-----	-----	-----	1.81	10	1.809	1
501	-----	-----	-----	-----	-----	-----	-----	-----	1.732	2
131	-----	-----	1.67	25	-----	-----	-----	-----	1.661	11
511	1.65	40	1.65	12	-----	-----	1.64	10	1.651	7
222	1.61	100	1.61	100	1.61	90	1.61	100	1.617	88
402	-----	-----	-----	-----	-----	-----	-----	-----	1.613	75
231	-----	-----	-----	-----	-----	-----	-----	-----	1.588	1
412	1.56	20	1.55	6	-----	-----	1.54	15	1.546	7
610	1.51	50	1.50	25	-----	-----	-----	-----	1.507	6
331	-----	-----	1.489	6	-----	-----	1.50	15	1.4858	7
521	1.46	40	1.465	31	1.463	20	1.46	30	1.4629	14
430	-----	-----	-----	-----	-----	-----	-----	-----	1.4415	3
113, 203	-----	-----	1.410	0	-----	-----	1.409	15	1.4086	4
422	-----	-----	-----	-----	-----	-----	-----	-----	1.3882	4
040	-----	-----	1.371	38	1.370	40	1.374	55	1.3686	21
620	1.36	80	1.362	75	1.361	20	1.354	75	1.3602	27
303	1.34	40	1.336	12	-----	-----	-----	-----	1.3349	5
313	1.30	70D	1.299	25	-----	-----	1.299	35	1.2973	10
123, 701	-----	-----	1.287	56	1.286	20	1.289	55	1.2861	13
531	1.26	70	-----	-----	-----	-----	-----	-----	1.2556	4
711, 223	-----	-----	1.253	62	1.253	20	1.254	55	1.2519	11
341, 432	1.21	40	1.208	50	-----	-----	1.218	<10	-----	-----
-----	-----	-----	-----	-----	-----	-----	1.208	45	1.2073	8
-----	-----	-----	-----	-----	-----	-----	1.198	<10	-----	-----
630	1.19	40D	-----	-----	-----	-----	1.188	10	1.1892	3
440	-----	-----	-----	-----	-----	-----	1.183	20	1.1831	3
042, 721	1.16	40	1.164	0	-----	-----	1.173	15	1.1643	2
503	-----	-----	-----	-----	-----	-----	-----	-----	1.1608	1
441	1.14	50	1.145	19	-----	-----	-----	-----	1.1429	4
513, 801	-----	-----	1.136	6	-----	-----	-----	-----	1.1361	3
004	1.11	50	1.107	50	-----	-----	-----	-----	1.1066	5
114, 333	1.08	60	-----	-----	-----	-----	-----	-----	1.0775	3
204	1.06	60	-----	-----	-----	-----	-----	-----	1.0688	4
523	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
151	1.06	20	-----	-----	-----	-----	-----	-----	1.0563	2
632	-----	-----	-----	-----	-----	-----	-----	-----	1.0475	2
304, 442	1.04	70	-----	-----	-----	-----	-----	-----	1.0434	10
802	-----	-----	-----	-----	-----	-----	-----	-----	1.0383	4
433, 640	-----	-----	-----	-----	-----	-----	-----	-----	1.0313	<1

Beryllium Aluminum Oxide (chrysoberyl), BeAl_2O_4 (orthorhombic)

<i>hkl</i>	----- British Museum		1942 Gjessing, Larsson and Major		1949 Foster and Royal		1949 Budnikov, Ayetikov, Dudavskij and Zvjagilskij		1959 National Bureau of Standards	
	Cu, 1.541 Å		Fe, 1.936 Å		Cu, 1.5405 Å		Cr, 2.2909 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
124, 812	1.02	20	-----	-----	-----	-----	-----	-----	1.0200	2
351	-----	-----	-----	-----	-----	-----	-----	-----	1.0067	2
224	-----	-----	-----	-----	-----	-----	-----	-----	1.0023	3
404	1.00	60	-----	-----	-----	-----	-----	-----	1.0011	3
703	-----	-----	-----	-----	-----	-----	-----	-----	0.9933	4
533	-----	-----	-----	-----	-----	-----	-----	-----	.9795	1
822	-----	-----	-----	-----	-----	-----	-----	-----	.9706	<1
252	-----	-----	-----	-----	-----	-----	-----	-----	.9610	<1
343	-----	-----	-----	-----	-----	-----	-----	-----	.9557	3
921	-----	-----	-----	-----	-----	-----	-----	-----	.9533	6
741	-----	-----	-----	-----	-----	-----	-----	-----	.9371	5
10·1·0	-----	-----	-----	-----	-----	-----	-----	-----	.9269	1
551	-----	-----	-----	-----	-----	-----	-----	-----	.9254	2
443	-----	-----	-----	-----	-----	-----	-----	-----	.9230	2
803	-----	-----	-----	-----	-----	-----	-----	-----	.9194	2
813	-----	-----	-----	-----	-----	-----	-----	-----	.9068	1
334, 452	-----	-----	-----	-----	-----	-----	-----	-----	.9057	1
832	-----	-----	-----	-----	-----	-----	-----	-----	.9024	2
650	-----	-----	-----	-----	-----	-----	-----	-----	.8976	1
260	-----	-----	-----	-----	-----	-----	-----	-----	.8958	1
614, 840	-----	-----	-----	-----	-----	-----	-----	-----	.8919	1
161	-----	-----	-----	-----	-----	-----	-----	-----	.8897	2
105	-----	-----	-----	-----	-----	-----	-----	-----	.8814	<1
434, 261	-----	-----	-----	-----	-----	-----	-----	-----	.8780	<1
153	-----	-----	-----	-----	-----	-----	-----	-----	.8757	1
015, 841	-----	-----	-----	-----	-----	-----	-----	-----	.8742	2
10·2·1	-----	-----	-----	-----	-----	-----	-----	-----	.8720	3
115, 552	}	-----	-----	-----	-----	-----	-----	-----	.8701	2
205		-----	-----	-----	-----	-----	-----	-----	.8656	1
10·0·2	-----	-----	-----	-----	-----	-----	-----	-----	.8606	7
044	-----	-----	-----	-----	-----	-----	-----	-----	.8584	12
624	-----	-----	-----	-----	-----	-----	-----	-----	.8551	2
10·1·2	-----	-----	-----	-----	-----	-----	-----	-----	.8521	2
305	-----	-----	-----	-----	-----	-----	-----	-----	.8467	2
353, 244	-----	-----	-----	-----	-----	-----	-----	-----		
11·0·1	}	-----	-----	-----	-----	-----	-----	-----	.8393	3
932		-----	-----	-----	-----	-----	-----	-----	.8304	7
262		-----	-----	-----	-----	-----	-----	-----	.8284	6
405		-----	-----	-----	-----	-----	-----	-----	.8272	6
842	-----	-----	-----	-----	-----	-----	-----	-----		
10·2·2	-----	-----	-----	-----	-----	-----	-----	-----	.8252	5
923	-----	-----	-----	-----	-----	-----	-----	-----	.8141	4
325	-----	-----	-----	-----	-----	-----	-----	-----	.8101	1
444	-----	-----	-----	-----	-----	-----	-----	-----	.8081	3
561	-----	-----	-----	-----	-----	-----	-----	-----	.8073	3
743	-----	-----	-----	-----	-----	-----	-----	-----	.8040	4
814	-----	-----	-----	-----	-----	-----	-----	-----	.7971	<1
135	-----	-----	-----	-----	-----	-----	-----	-----	.7937	3
515, 752	-----	-----	-----	-----	-----	-----	-----	-----	.7925	2
660, 851	-----	-----	-----	-----	-----	-----	-----	-----	.7886	5
12·0·0	-----	-----	-----	-----	-----	-----	-----	-----	.7836	1

Beryllium Aluminum Silicate (beryl), $\text{Be}_3\text{Al}_2(\text{SiO}_3)_6$ (hexagonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-0079	8.1 3.33 2.92	Copper	British Museum.
2-0080	7.90 3.25 2.87	Copper	Wyandotte Chemical Co., Wyandotte, Mich.
3-0463 3-0464	3.28 2.88 0.81	Copper	Schiebold [1] 1935 (synthetic).
3-0480 3-0481	3.25 2.88 0.81	Copper	Schiebold [1] 1935 (natural).

Card #3-0462 reports d -spacings to 1.22; otherwise it has the same data as cards #3-0463 and 3-0464. Therefore, this card is not used in the comparison table.

Additional published patterns

Source	Radiation
Norrish [2] 1947	Copper K_α

NBS sample. The sample of beryl was obtained from Royalston, Mass. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of iron, sodium, and zinc; and 0.001 to 0.01 percent each of magnesium, manganese, strontium, and titanium.

The sample is colorless and optically negative. The refractive indices are $N_o = 1.579$ and $N_e = 1.572$.

Interplanar spacings and intensity measurements. The d -values reported by the British Museum and by the Wyandotte Chemical Co. were converted from kX to angstrom units. The three patterns reported by Schiebold were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
British Museum	100	211	110, 002
Wyandotte Chemical Co.	100	112	211
Schiebold (synthetic)	112	211	110, 002
Schiebold (natural)	112	211	110, 002
Norrish	100	112	211
National Bureau of Standards	211	112	100

Structural data. Bragg and West [3] in 1926 determined that beryl has the space group $P6/mmc$ (No. 192) and $2[\text{Be}_3\text{Al}_2(\text{SiO}_3)_6]$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	c
		A	A
1926	Bragg and West [3]	9.23	9.19
1935	Schiebold [1] (synthetic)	9.235	9.203
1935	Schiebold [1] (natural)	9.415	9.226
1935	Schiebold [1] (natural)	9.231	9.188
1947	Norrish [2]	9.188	9.189
1951	Belov and Matveeva [4]	9.206	9.205
1959	National Bureau of Standards	9.215	9.192 at 25° C

The density of beryl calculated from NBS lattice constants is 2.640 g/cm^3 at 25°C .

References

- [1] E. Schiebold, Verleichenende Untersuchungen an natuerlichen und synthetischen Smaragdkristallen, *Z. Krist.* **92**, 435-473 (1935).
- [2] K. Norrish, X-ray study of West Australian beryl, *J. Roy. Soc. W. Aust.* **34**, 1-16 (1947).
- [3] W. L. Bragg and J. West, The structure of beryl, $\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$, *Proc. Roy. Soc.* **111A**, 691-714 (1926).
- [4] N. V. Belov and R. G. Matveeva, The determination of parameters of beryl structure by a method of partial projections, *Trudy Inst. Krist. Akad. Nauk S. S. S. R.* **6**, 69 (1951).

Beryllium Aluminum Silicate (beryl), $\text{Be}_3\text{Al}_2(\text{SiO}_3)_6$ (hexagonal)

<i>hkl</i>	----- British Museum		----- Wyandotte Chemical Co.		1935 Schiebold (synthetic)		1935 Schiebold (natural)		1947 Norrish		1959 National Bureau of Standards	
	Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
----- 100 -----	<i>A</i> 9.4 8.1 5.2	40 100 40	<i>A</i> 7.92	100	<i>A</i> ----- -----	----- ----- -----	<i>A</i> ----- -----	----- ----- -----	<i>A</i> 7.93	s	<i>A</i> 7.98	93
110 002	4.7	60	4.61	40	4.64	s	4.60	s	4.60	m	4.60	51
200 102	4.46 4.08	20 60	----- 4.01	----- 50	----- 4.04	----- s	----- 3.99	----- s	----- 3.96	----- m	----- 3.99	----- 46
----- ----- -----	3.68 3.33	50 80	----- -----	----- -----	----- -----	----- -----	----- -----	----- -----	----- -----	----- -----	----- -----	----- -----
112 210 202	3.24 3.06	20 60	3.26 3.01	100 30	3.29 3.05	vs s	3.26 3.02	vs s	3.25 3.01	s m	3.254 3.015	95 34
211 300	2.93	80	2.88	100	2.89 2.71	vs w	2.89	vs	2.86 2.65	s ⁻ vw	2.867 2.660	100 2
212	2.56	50	2.53 2.37	40 10	2.55	s	2.54	s	2.51	m	2.523	30
220 302 004	2.34	40	2.30	10	2.32	ms	2.30	ms	2.289	w	2.293	10
310 104	2.23	40	----- 2.20	----- 20	2.22	m	2.21	m	----- 2.203	----- w	2.213 2.208	6 2
311 222 114	2.16 2.09 2.02	40 20 60	2.14	20	2.16 2.08	s mw	2.15 2.06	s mw	2.142	w	2.152 2.060 2.056	14 3 4
312 204	1.99	20	1.98	40	2.00	s ⁻	1.99	s	1.986	w-m	1.9926	22
320 402	1.86 1.81	20 50	1.92	20	----- 1.85	----- w	----- 1.84	----- w	1.922 1.821	vw vw	----- 1.8308	----- 6
321 313 304	1.76 1.72	60 40	1.79 1.73	30 50	1.81 1.75	ms s	1.80 1.74	ms s	1.784 1.733	w w-m	1.7954 1.7397	17 19
411 322	----- -----	----- -----	1.71	20	1.72	m	1.71	m	----- 1.700	----- w	1.7110 1.7007	12 2
412 224	1.64 1.61	60 50	1.67 1.62	10 30	----- 1.64	----- s	----- 1.63	----- s	----- 1.622	----- w	----- 1.6265	----- 17
500 314	1.58	50	1.59	10	1.60	m	1.61	m	1.589	vw	1.5953	6
323 215 330	----- 1.55	----- 40	1.57	20	1.58	m	1.57	m	----- 1.561	----- vw	1.5710 1.5690	9 7
006 413	1.53	60	-----	-----	1.54	mw	1.53	mw	1.528	vw	1.5349 1.5320	5 7
----- ----- -----	----- ----- -----	----- ----- -----	1.51	40	1.52	s	1.52	s	1.507	w	1.5138	15
421 332 116	1.47 1.44	50 60	----- 1.45	----- 20	----- 1.46	----- ms	----- 1.46	----- ms	----- 1.450	----- w	1.4882 1.4566 1.4535	1 9 10
510, 422 324, 206	-----	-----	1.43	30	1.44	s	1.43	s	1.429	w	1.4324	13
315	1.41	20	1.41 1.40	10 10	1.42	vw	-----	-----	-----	-----	1.4148	1

Beryllium Aluminum Silicate (beryl), $\text{Be}_3\text{Al}_2(\text{SiO}_6)_3$ (hexagonal)

<i>hkl</i>	----- British Museum		----- Wyandotte Chemical Co.		1935 Schiebold (synthetic)		1935 Schiebold (natural)		1947 Norrish		1959 National Bureau of Standards	
	Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
512	<i>A</i>		<i>A</i>		<i>A</i>		<i>A</i>		<i>A</i>		<i>A</i>	
216	1.38	50	1.37	20	1.34	s	1.33	s	1.362	w	1.3682	7
600	-----	-----	1.33	20	1.34	w	-----	-----	-----	-----	1.3656	6
430	-----	-----	-----	-----	1.32	vw	1.33	vw	1.328	vvw	1.3306	<1
504	-----	-----	-----	-----	1.30	vw	1.30	vw	-----	-----	1.3117	<1
513	-----	-----	-----	-----	1.28	s	1.28	s ⁻	-----	-----	1.2977	<1
325	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
520	-----	-----	1.27	40	1.27	s	1.27	s ⁻	1.272	w-m	1.2774	11
602, 334	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
415	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
521	-----	-----	1.26	40	1.24	vw	1.23	vw	1.257	w-m	1.2657	13
432	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	1.2628	9
424	-----	-----	-----	-----	1.22	w	1.22	w	-----	-----	1.2170	2
610	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
611	-----	-----	1.20	40	1.21	s	1.21	s ⁻	1.200	w-m	1.2062	10
433	-----	-----	-----	-----	1.19	mw	1.18	mw	-----	-----	1.2041	9
217	-----	-----	-----	-----	-----	-----	-----	-----	1.176	vvw	1.1795	1
523	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
440, 604	-----	-----	-----	-----	1.15	ms	1.15	ms	-----	-----	1.1511	4
416	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
008	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
700	-----	-----	-----	-----	1.14	m	1.14	m	1.148	vw	1.1490	4
434	-----	-----	-----	-----	-----	-----	-----	-----	1.134	vw	1.1396	3
442	-----	-----	-----	-----	1.12	ms	1.12	ms	1.114	vw	1.1173	7
524	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
620	-----	-----	-----	-----	1.11	mw	1.11	mw	1.104	vvw	1.1066	<1
702	-----	-----	-----	-----	1.09	m	1.09	ms	1.083	vvw	1.0848	2
336	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
426	-----	-----	-----	-----	1.07	ms	1.07	ms	1.073	vvw	1.0752	4
218	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
533, 435	-----	-----	-----	-----	1.05	s	1.05	s	1.065	vvw	1.0683	5
327	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
525	-----	-----	-----	-----	1.03	w	1.03	w	1.046	vw	1.0493	6
417	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	1.0485	4
623	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	1.0405	<1
712	-----	-----	-----	-----	1.02	m	1.02	m	1.028	vvw	1.0297	<1
444	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
541	-----	-----	-----	-----	1.01	w	1.01	w	1.012	vvw	1.0157	3
615	-----	-----	-----	-----	(a)		(b)		(c)			

^a Twenty-nine additional lines are omitted.

^b Twenty-one additional lines are omitted.

^c Fourteen additional lines are omitted.

Bismuth Oxyiodide, BiOI (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-0634	3.02 9.1 2.28	Copper	British Museum.

Additional published patterns. None.

NBS sample. The sample of bismuth oxyiodide was prepared at NBS by reacting Bi_2O_3 with con-

centrated HI followed by prolonged hydrolysis of the product in boiling water. The X-ray pattern was improved by heating the material in air for 2 hr at 450°C . Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of nickel; and 0.001 to 0.01 percent each of aluminum, cobalt, iron, and silicon.

The color of the sample was dark red-orange. The indices of refraction were too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements.

The d -values reported by the British Museum were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

<i>hkl</i>	----- British Museum		1959 National Bureau of Standards		<i>hkl</i>	----- British Museum		1959 National Bureau of Standards	
	Cu, 1.541 Å		Cu, 1.5405 Å at 25° C			Mo, 1.541 Å		Cu, 1.5405 Å at 25°	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>		<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
001	<i>A</i> 9.1	80	<i>A</i> 9.15	22	312	1.216	20	1.2176	2
002	4.51	60	4.58	7	206	-----	-----	1.2121	<1
101	-----	-----	3.661	3	224	1.204	20	1.2017	2
102	3.02	100	3.011	100	117	1.186	10	1.1860	1
110	2.82	60	2.824	53	216	1.161	50	1.1597	1
111	-----	-----	2.699	3	304	-----	-----	1.1502	<1
103	2.42	40	2.424	10	008	-----	-----	1.1436	<1
112	-----	-----	2.403	7	225	-----	-----	1.1181	<1
004	2.28	80	2.287	9	314	1.112	60D	1.1058	4
113	-----	-----	2.072	2	321	}-----	-----	1.0993	1
200	} 1.98	60	1.997	24	108			1.0936	<1
104			1.985	10	207	-----	-----	1.0768	5
201			1.952	3	322	} 1.078	50	{ 1.0601	<1
202	} 1.82	40	1.829	3	305				
005			-----	-----	118	} 1.058	40	{ 1.0548	1
114	1.77	60	1.778	15	217				
212	} 1.66	70	1.664	32	323	-----	-----	1.0416	1
105			-----	-----	315	} 1.039	40	{ 1.0393	1
213			1.541	6	226			{ 1.0363	1
115	1.537	50D	1.5359	3	009	1.019	20		
006	-----	-----	1.5246	3	306	} 1.001	20B	{ 1.0028	<1
204	1.505	40	1.5045	6	400				
106	1.427	70	1.4244	4	401	-----	-----	.9925	<1
220	-----	-----	1.4120	6	208	-----	-----	.9852	1
214	1.408	50	1.4078	4	109	0.969	40	.9728	1
221	-----	-----	1.3957	<1	316	}-----	-----	.9632	1
222	}-----	-----	1.3495	4	411			.9566	<1
205			1.3422	4	218	-----	-----		
116			1.309	20	1.3073	1	119	-----	-----
302	} 1.281	40	1.2786	3	325	}-----	-----	.9414	<1
215			1.2634	3	412				
310			1.2424	2	330				
107	1.242	60	1.2200	<1	-----	-----	-----	-----	-----
303	-----	-----	-----	-----	-----	-----	-----	-----	-----

Pattern	1	2	3
British Museum.....	102	001	004
National Bureau of Standards..	102	110	212, 105

Structural data. Bannister and Hey [1] in 1935 determined that bismuth oxyiodide has lead fluo-chloride-type structure, the space group $P4/nmm$ (No. 129), and 2(BiOI) per unit cell.

Two unit-cell measurements have been converted from kX to angstrom units for comparison with NBS values.

The density of bismuth oxyiodide calculated from NBS lattice constants is 8.006 g/cm³ at 25° C.

Cadmium Bromide, CdBr₂ (trigonal)

ASTM cards. None. Card number 3-0088 is a different form.

Additional published patterns

Source	Radiation
Pinsker [1] 1942.....	Electron diff.

NBS sample. The sample of cadmium bromide was obtained from the City Chemical Corp., New York, as a hydrate. The sample was heated to 550° C to dehydrate and to sharpen the pattern. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of aluminum, iron, and silicon.

The sample was colorless. The indices of refraction were too high to be measured by the oil immersion method.

Interplanar spacings and intensity measurements. The d -values reported by Pinsker have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Pinsker.....	110	104	113
National Bureau of Standards.....	003	110	104

		a	c
		A	A
1935	Bannister and Hey [1].....	4.02	9.16
1941	Sillén [2].....	3.992	9.146
1959	National Bureau of Standards.....	3.994	9.149 at 25° C

References

- [1] F. A. Bannister and M. H. Hey, The crystal-structure of the bismuth oxyhalides, *Mineralog. Mag.* **24**, 49-58 (1935).
- [2] L. G. Sillén, X-ray studies on BiOCl, BiOBr and BiOI, *Svensk Kem. Tidsskr.* **53**, 39-43 (1941).

hkl hex.	1942 Pinsker		1959 National Bureau of Standards	
	Electron Diffraction		Cu, 1.5405 Å at 25° C	
	d	I	d	I
	A		A	
003	-----	-----	6.27	100
101	3.42	25	3.40	10
006	-----	-----	3.14	8
104	2.80	70	2.785	19
015	-----	-----	2.546	3
107	-----	-----	2.123	2
009	-----	-----	2.094	7
110	2.00	100	1.993	39
018	1.94	36	1.947	6
113	1.91	70	1.899	15
1·0·10	1.70	14	1.654	3
024	1.62	70	1.621	2
0·0·12	-----	-----	1.570	9
0·1·11	-----	-----	1.5345	1
119	1.44	14	1.4439	4
208	1.40	18	1.3917	5
1·0·13	-----	-----	1.3366	1
0·0·15	1.26	36	1.2561	5
1·1·12	1.24	50	1.2334	10
-----	1.15	18	-----	-----
128	1.14	11	1.1413	3
1·0·16	1.13	11	1.1146	2
1·1·15	-----	-----	1.0625	2
0·1·17	-----	-----	1.0551	1
0·0·18	-----	-----	1.0466	1
0·2·16	-----	-----	0.9734	2
312	-----	-----	.9524	2
1·0·19	-----	-----	.9381	1
134	-----	-----		
1·2·14	-----	-----		
3·0·12	-----	-----	.9280	3
315	-----	-----	.9265	3
1·1·18	-----	-----	.9087	1
0·1·20	-----	-----	.8741	3
2·1·16	-----	-----		

Structural data. Pinsker [1] in 1942 determined that this form of cadmium bromide has the cadmium chloride-type structure, the space group $R\bar{3}m$ (No. 166) and $3(\text{CdBr}_2)$ per unit hexagonal cell or $1(\text{CdBr}_2)$ per unit rhombohedral cell. Several other forms of cadmium bromide have been reported in the literature by Pinsker [1], Bijvoet and Nieuwenkamp [2], and Hägg, Kiessling, and Linden [3].

Lattice constants

		<i>a</i>	<i>c</i>
1942	Pinsker [1]-----	<i>A</i>	<i>A</i>
1943	Hägg, Kiessling, and Linden [3]-----	4.01	18.88
1959	National Bureau of Standards-----	3.99	18.78
		3.985	18.841 at 25° C

The density of cadmium bromide calculated from the NBS lattice constants is 5.203 g/cm³ at 25° C.

References

- [1] Z. G. Pinsker, Electron diffraction of the structure of CdBr_2 , J. Phys. Chem. USSR 16, 1-12 (1942).
- [2] J. M. Bijvoet and W. Nieuwenkamp, Kürzere Originalmitteilungen und Notizen, Die $\langle\langle\text{Wechselstruktur}\rangle\rangle$ von CdBr_2 , Z. Krist. 86A, 466-470 (1933).
- [3] G. Hägg, R. Kiessling, and E. Linden, The crystal structure of CdBr_2 and CdI_2 , Arkiv Kemi, Mineral. Geol. No. 4 16B, 1 (1943).

Cadmium Chloride, CdCl_2 (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0169	5.8 2.65 3.28	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Structural data. Pauling [2] in 1929 determined that cadmium chloride has the space group $R\bar{3}m$ (No. 166) and $3(\text{CdCl}_2)$ per unit hexagonal cell or $1(\text{CdCl}_2)$ per unit rhombohedral cell. Cadmium chloride is used as a structure type and shown to be isomorphous with MgCl_2 , ZnCl_2 , MnCl_2 , and FeCl_2 in 1927 [3]. The unit-cell measurements have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		<i>a</i>	<i>c</i>
1930	Pauling and Hoard [4]-----	<i>A</i>	<i>A</i>
1941	Pinsker and Tatarinova [5]--	3.86	17.50
1959	National Bureau of Standards-----	3.85	17.46
		3.844	17.489 at 25° C

Additional published patterns. None.

NBS sample. The sample of cadmium chloride was obtained from Fisher Scientific Co. Spectrographic analysis shows the following impurities: 0.0001 to 0.001 percent each of aluminum and silicon.

The sample is colorless and optically positive. The indices of refraction are $N_o=1.681$ and $N_e=1.719$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel-----	003	104	101
National Bureau of Standards-----	003	104	101

The density of cadmium chloride calculated from the NBS lattice constants is 4.080 g/cm³ at 25° C.

Cadmium Chloride, CdCl₂ (trigonal)

<i>hkl</i> hex.	1938		1959	
	Hanawalt, Rinn, and Frevel		National Bureau of Standards	
	Mo, 0.7107 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	<i>A</i>		<i>A</i>	
003	5.8	100	5.85	100
101	3.29	60	3.27	70
102	-----	-----	3.114	11
006	-----	-----	2.925	3
104	2.66	80	2.648	90
015	2.40	25	2.412	28
107	1.99	12	1.998	18
009	-----	-----	1.943	10
110	1.92	40	1.922	31
-----	1.87	4	-----	-----
113	1.83	50	1.826	54
021	1.66	8	1.658	10
202	-----	-----	1.632	3
024	1.56	12	1.556	17
205	1.50	6	1.503	6
0·0·12	} 1.451	4	{ 1.4578	8
0·1·11			{ 1.4353	7
027			1.3855	6
119			1.3666	7
208			1.3245	8
211	1.258	6	1.2550	6
1·0·13	-----	-----	1.2473	2
214	1.214	8	1.2092	14
125	1.188	4	1.1846	4
0·0·15	1.166	6	1.1662	9
1·1·12	-----	-----	1.1616	3
2·0·11	-----	-----	1.1500	1
217	1.129	2	1.1239	1
300	1.118	2	1.1097	6
128	1.096	6	1.0905	10
1·0·16	-----	-----	1.0385	6
1·1·15	-----	-----	0.9971	6
1·2·11	-----	-----	.9867	4
309	-----	-----	.9632	7
220	-----	-----	.9612	5
223	-----	-----	.9483	4
131	-----	-----	.9220	4
2·1·13	-----	-----	.9190	4
0·2·16	-----	-----	.9137	3
134	-----	-----	.9036	9
1·0·19	-----	-----	.8871	2
3·0·12	-----	-----	.8829	8
137	-----	-----	.8657	4
318	-----	-----	.8507	7
2·1·16	-----	-----	.8253	8
404	-----	-----	.8176	5
3·0·15	-----	-----	.8036	4
2·2·12	-----	-----	.8024	5

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10**, 457-512 (1938).
- [2] L. Pauling, On the crystal structure of the chlorides of certain bivalent elements, Proc. Nat. Acad. Sci. U.S. **15**, 709-712 (1929).
- [3] G. Bruni and A. Ferrari, Z. physik. Chem. **130**, 488-494 (1927).
- [4] L. Pauling and J. L. Hoard, The crystal structure of cadmium chloride, Z. Krist. **74**, 546-551 (1930).
- [5] Z. G. Pinsker and L. I. Tatarinova, Electronographic investigation of cadmium chloride, Acta Physicochim. U.S.S.R. **14**, 737-744 (1941).

Calcium Aluminate 12:7, $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$ (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-0912	2.69	Molybdenum Copper	Harrington [1] 1927. Brownmiller and Bogue [2] 1932.
	5.04		
	2.44		
3-0149	4.85	Copper	Büssem and Eitel [3] 1936.
	2.67		
	2.98		
1-1057	2.68	Molybdenum	Hanawalt, Rinn, and Frevel [4] 1938.
	4.95		
	2.44		

The three ASTM cards above are reported as $5\text{CaO} \cdot 3\text{Al}_2\text{O}_3$; according to Büssem and Eitel [3] and to Thorvaldson and Schneider [5] the formula should be $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$.

Additional published patterns. None.

NBS sample. The sample of calcium aluminate was prepared by the Portland Cement Association Fellowship at NBS. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of sodium, silicon, and strontium; 0.01 to 0.1 percent each of iron and magnesium; and 0.001 to 0.01 percent each of copper, manganese, and molybdenum.

The sample is colorless. The index of refraction could not be determined because the sample was too fine-grained.

Interplanar spacings and intensity measurements. The d -values reported by Harrington, by Brownmiller and Bogue, and by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units and the d -values reported by Büssem and Eitel were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Harrington.....	420	422	521
Brownmiller and Bogue.....	420	400	422
Hanawalt, Rinn, and Frevel.....	420	211	422
Büssem and Eitel.....	211	420	422
National Bureau of Standards.....	420	211	422

Structural data. Büssem and Eitel [3] in 1936, by consideration of the density, came to the conclusion that what was formerly called $5\text{CaO} \cdot 3\text{Al}_2\text{O}_3$ was in fact $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$. They then found that the space group was $I43d$ (No. 220), with $2(12\text{CaO} \cdot 7\text{Al}_2\text{O}_3)$ per unit cell. $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$ is used as a structure type.

The Büssem and Eitel unit-cell measurement has been converted from kX to angstrom units for comparison with the NBS values. The Harrington value was obtained from the powder pattern rather than his reported value.

Lattice constants

		A
1927	Harrington [1].....	11.99
1936	Büssem and Eitel [3].....	11.97
1959	National Bureau of Standards.....	11.982 at 25° C

The density of this compound, using the formula $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$, calculated from the NBS lattice constant is 2.676 g/cm^3 at 25°C .

References

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- [2] L. T. Brownmiller and R. H. Bogue, The system $\text{CaO}-\text{Na}_2\text{O}-\text{Al}_2\text{O}_3$, *Am. J. Sci.* **23**, 501-524 (1932).
- [3] W. Büssem and A. Eitel, Die Struktur des Pentacalcium-trialuminats, *Z. Krist.* **95**, 175-188 (1936).
- [4] J. D. Hanawalt, H. W. Rinn and L. K. Frevel, Chemical analysis by X-ray diffraction, *Ind. Eng. Chem., Anal. Ed.* **10**, 457-512 (1938).
- [5] T. Thorvaldson and W. G. Schneider, The composition of "5:3" calcium aluminate, *Can. J. Research* **19B**, 109-115 (1941).

Calcium Aluminate 12:7, 12CaO · 7Al₂O₃ (cubic)

<i>hkl</i>	1927				1932				1936				1938				1959			
	Harrington				Brownmiller and Bogue				Büsem and Eitel				Hanawalt, Rinn, and Frevel				National Bureau of Standards			
	Mo, 0.7107 Å				Mo, 0.7107 Å				Cu, 1.537 Å				Mo, 0.7107 Å				Cu, 1.5405 Å at 25° C			
	<i>d</i>	<i>I</i>	<i>a</i>		<i>d</i>	<i>I</i>	<i>a</i>		<i>d</i>	<i>I</i>	<i>a</i>		<i>d</i>	<i>I</i>	<i>a</i>		<i>d</i>	<i>I</i>	<i>a</i>	
211	A	---	A	---	A	---	A	---	A	>100	11.86	A	A	67	12.2	A	A	95	11.98	A
220	---	---	---	---	---	---	---	---	4.84	7	11.23	---	4.96	---	---	---	4.89	4	11.98	---
310	---	---	---	---	3.78	m	11.95	---	4.23	17	11.96	---	---	---	---	---	4.24	14	11.98	---
321	3.21	30	12.0	m	3.19	m	11.94	---	3.77	24	11.92	---	---	---	---	---	3.79	25	11.99	---
400	3.04	40	12.2	s	2.99	s	11.96	---	3.20	49	11.97	---	3.20	23	12.0	---	3.204	44	11.99	---
420	2.70	100	12.1	vs	2.68	vs	11.96	---	2.98	---	11.91	---	3.02	---	12.1	---	2.998	---	---	---
332	---	---	---	m	2.56	m	12.01	---	2.67	97	11.93	---	2.69	100	12.0	---	2.680	100	11.99	---
422	2.45	80	12.0	s	2.44	s	12.01	---	2.54	16	11.91	---	---	---	---	---	2.556	17	11.99	---
510	---	---	---	m	2.34	m	11.93	---	2.44	52	11.93	---	2.44	50	12.0	---	2.447	52	11.99	---
521	2.19	80	12.00	s	2.184	s	11.96	---	2.34	16	11.95	---	---	---	---	---	2.350	9	11.98	---
530	---	---	---	w	2.059	w	12.01	---	2.186	46	11.97	---	2.19	50	12.0	---	2.189	40	11.988	---
611	1.949	70	12.01	s	1.947	s	12.00	---	2.049	6	11.95	---	---	---	---	---	2.054	8	11.979	---
---	---	---	---	w	1.910	w	---	---	1.938	35	11.95	---	1.94	---	---	---	1.945	28	11.989	---
541	---	---	---	w	1.850	w	11.99	---	---	---	11.95	---	---	---	---	---	---	---	---	---
---	---	---	---	vw	1.804	vw	---	---	1.844	5	---	---	---	---	---	---	1.850	6	11.982	---
631	---	---	---	w	1.768	w	11.97	---	---	---	11.96	---	---	---	---	---	---	---	---	---
444	1.728	40	11.97	m	1.731	m	11.99	---	1.764	5	11.96	---	---	---	---	---	1.767	5	11.982	---
710	---	---	---	w	1.697	w	12.00	---	1.724	11	11.94	---	1.73	13	12.0	---	1.730	11	11.987	---
640	1.663	60	11.99	s	1.663	s	11.99	---	1.689	7	11.94	---	---	---	---	---	1.695	6	11.983	---
721	---	---	---	m	1.632	m	11.99	---	1.658	35	11.96	---	1.66	42	12.0	---	1.662	27	11.985	---
642	1.603	60	12.00	s	1.602	s	11.96	---	1.628	11	11.96	---	---	---	---	---	1.630	8	11.982	---
---	---	---	---	w	1.557	w	---	---	1.597	40	11.95	---	1.59	50	11.9	---	1.601	31	11.982	---
732	1.523	20	11.99	m	1.523	m	11.99	---	1.539	9	---	---	---	---	---	---	---	---	---	---
800	1.501	20	12.01	w	1.496	w	11.97	---	---	---	11.98	---	1.52	13	12.0	---	1.522	5	11.982	---
811	---	---	---	m	1.475	m	11.98	---	1.497	7	11.98	---	---	---	---	---	1.498	5	11.985	---
831	1.397	60	12.02	s	1.475	m	---	---	1.471	9	11.95	---	1.481	10	12.03	---	1.475	6	11.981	---
752	---	---	---	vw	1.393	s	11.98	---	---	---	11.97	---	---	---	---	---	---	---	---	---
840	1.345	20	12.03	w	1.356	vw	11.98	---	1.391	22	---	---	1.398	27	12.03	---	1.393	16	11.983	---
842	1.313	30	12.03	m	1.339	w	11.98	---	---	---	---	---	1.347	10	12.05	---	1.356	3	11.976	---
921	---	---	---	vw	1.308	m	11.99	---	---	---	---	---	1.312	17	12.02	---	1.340	6	11.983	---
---	---	---	---	vw	1.293	vw	---	---	---	---	---	---	---	---	---	---	1.307	7	11.982	---
664	---	---	---	w	1.277	w	11.98	---	---	---	---	---	---	---	---	---	1.292	5	11.982	---
930	1.263	20	11.98	w	1.263	w	11.98	---	---	---	---	---	---	---	---	---	---	---	---	---
932	1.241	10	12.03	w	1.236	w	11.98	---	---	---	---	---	1.264	---	11.99	---	1.277	4	11.983	---
941	1.212	20	12.00	w	1.209	w	11.97	---	---	---	---	---	---	10	---	---	1.263	3	11.979	---
---	---	---	---	vw	1.189	vw	---	---	---	---	---	---	1.211	---	11.99	---	1.236	4	11.980	---
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

Calcium Aluminate 12:7, CaO·7Al₂O₃ (cubic)

<i>hkl</i>	1927			1932			1936			1938			1959		
	Harrington Mo, 0.7107 Å			Brownmiller and Bogue Mo, 0.7107 Å			Bussem and Eitel Cu, 1.537 Å			Hanawalt, Rinn, and Frevel Mo, 0.7107 Å			National Bureau of Standards Cu, 1.5405 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
10·2·0	A	10	A	A	w	A	A	---	---	A	10	---	A	1	A
10·3·1	1.180	10	12.03	1.173	vw	11.96	---	---	---	1.176	7	---	1.175	2	11.984
10·4·0	1.144	30	12.00	1.142	m	11.98	---	---	---	1.143	13	---	1.143	6	11.985
10·4·2	1.115	20	12.01	1.112	w	11.98	---	---	---	1.114	3	---	1.112	4	11.981
11·1·0	1.091	---	11.95	1.093	w	11.97	---	---	---	1.093	---	---	1.094	2	11.980
	---	---	---	1.086	---	12.00	---	---	---	---	---	---	1.085	---	11.982
11·2·1	1.066 (^a)	20	11.97	1.068 (^b)	w	11.99	---	---	---	---	---	---	---	---	---
Average value of last five lines			11.99	---	---	11.98	---	---	11.97	---	---	---	---	---	11.982

^a Eleven additional lines were omitted.
^b Twelve additional lines were omitted.

Calcium Iron Silicate (andradite),
Ca₃Fe₂Si₃O₁₂ (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
3-0814	2.69 1.61 3.01	Copper	Flint, McMurdie, and Wells [1] 1941.
3-1135	1.61 1.67 1.07	Copper	Menzer [2] 1929.

Additional published patterns. None.

NBS sample. The sample of calcium iron silicate was prepared at NBS by hydrothermal synthesis at 850° C and 20,000 psi using a cold seal bomb. The starting material was a gel made from nitrates of ferric iron and calcium, and ethyl orthosilicate. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, chromium, magnesium, molybdenum, and strontium; 0.0001 to 0.001 percent each of copper, potassium, sodium, nickel, and rubidium.

The sample had a brownish-reddish color. The index of refraction was 1.887.

Interplanar spacings and intensity measurements. The *d*-values reported by Flint, McMurdie, and Wells were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Flint, McMurdie, and Wells-----	420	642	400
Menzer-----	642	420	400
National Bureau of Standards-----	420	400	642

Structural data. Menzer [2] in 1929 determined that andradite was a member of the garnet group, the space group Ia3d (No. 230) and 8(Ca₃Fe₂Si₃O₁₂) per unit cell.

The unit-cell measurement reported by Zedlitz was converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		<i>a</i>
1929	Menzer [2]-----	12.044
1935	Zedlitz [3]-----	12.043
1941	Flint, McMurdie, and Wells [1]-----	12.04
1959	National Bureau of Standards-----	12.059 at 25° C

Calcium Iron Silicate (andradite), $\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$ (cubic)

<i>hkl</i>	1929			1941			1959		
	Menzer			Flint, McMurdie, and Wells			National Bureau of Standards		
	Cu, 1.5405 Å			Cu, 1.5405 Å			Cu, 1.5405 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
220	4.275	15	12.09	4.25	40	12.0	4.263	13	12.058
400	3.029	59	12.12	3.02	80	12.1	3.015	60	12.060
420	2.709	75	12.11	2.69	100	12.0	2.696	100	12.058
332	2.595	13	12.17	2.57	20	12.0	2.571	13	12.061
422	2.465	50	12.08	2.45	80	12.0	2.462	46	12.063
510	2.379	20	12.13	2.35	40	12.0	2.365	17	12.060
521	2.212	13	12.12	2.20	40	12.0	2.202	17	12.059
611	1.963	28	12.10	1.95	60	12.0	1.9564	24	12.060
620	1.914	17	12.10	1.89	40	12.0	1.9068	10	12.060
-----	1.859	8	-----	-----	-----	-----	-----	-----	-----
-----	1.790	22	-----	-----	-----	-----	-----	-----	-----
444	1.739	13	12.05	1.74	20	12.0	1.7406	8	12.059
-----	1.704	8	-----	-----	-----	-----	-----	-----	-----
640	1.675	50	12.08	1.67	60	12.0	1.6728	25	12.063
721	1.645	10	12.09	-----	-----	-----	1.6412	2	12.060
642	1.613	100	12.07	1.61	100	12.0	1.6112	59	12.057
800	1.511	22	12.09	1.51	40	12.1	1.5073	13	12.058
-----	1.458	10	-----	-----	-----	-----	-----	-----	-----
822	1.425	13	12.10	-----	-----	-----	1.4213	3	12.060
840	1.349	45	12.07	1.35	60	12.1	1.3483	13	12.060
842	1.316	45	12.06	1.31	60	12.0	1.3157	18	12.059
664	1.285	45	12.06	-----	-----	-----	1.2856	12	12.060
844	1.243	7	12.18	1.25	60	12.1	1.2309	3	12.060
941	1.219	17	12.07	1.21	20	12.0	1.2182	4	12.060
-----	1.183	12	-----	-----	-----	-----	-----	-----	-----
-----	1.152	5	-----	-----	-----	-----	-----	-----	-----
-----	1.130	5	-----	-----	-----	-----	-----	-----	-----
10·4·0	1.119	53	12.06	1.11	60	12.0	1.1195	25	12.057
10·4·2	1.100	53	12.05	-----	-----	-----	1.1008	15	12.059
880	1.065	50	12.06	-----	-----	-----	1.0659	12	12.059
-----	1.031	7	-----	-----	-----	-----	-----	-----	-----
12·0·0	1.005	25	12.06	-----	-----	-----	1.0049	7	12.059
12·2·0	0.990	25	12.05	-----	-----	-----	0.9912	6	12.058
12·2·2	.978	67	12.06	-----	-----	-----	.9781	17	12.059
11·6·3	.934	12	12.04	-----	-----	-----	.9359	4	12.058
12·6·0	-----	-----	-----	-----	-----	-----	.8988	7	12.059
12·6·2	-----	-----	-----	-----	-----	-----	.8889	5	12.058
888	-----	-----	-----	-----	-----	-----	.8703	4	12.059
14·2·0	-----	-----	-----	-----	-----	-----	.8527	2	12.060
12·8·0	-----	-----	-----	-----	-----	-----	.8361	3	12.058
14·4·0	-----	-----	-----	-----	-----	-----	.8282	6	12.059
14·4·2	-----	-----	-----	-----	-----	-----	.8205	15	12.059
Average value of last five lines			12.05	-----	-----	12.0	-----	-----	12.059

References

- [1] E. P. Flint, H. F. McMurdie, L. S. Wells, Hydrothermal and X-ray studies of the garnet-hydrogarnet series and the relationship of the series to hydration products of Portland cement, *J. Research Nat. Bur. Standards* **26**, 13-33 (1941).
- [2] G. Menzer, Die kristallstruktur der granate, *Z. Krist. Mineral.* **69**, 300-396 (1929).
- [3] O. Zedlitz, Über titanhaltige kalkeisengranate, II, *Zentr. Mineral. Geol., abt. A*, 68-78 (1935).

The density of andradite calculated from the NBS lattice constant is 3.849 g/cm³ at 25° C.

Cesium Bromotellurate, Cs₂TeBr₆ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium bromotellurate was prepared at the NBS from bromotelluric acid and cesium bromide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of potassium, sodium, and rubidium; and 0.001 to 0.01 percent each of aluminum, calcium, chromium, iron, magnesium, manganese, molybdenum, silicon, and vanadium.

The color of the sample is deep orange. The index of refraction was not obtained because the sample was too highly colored.

Interplanar spacings and intensity measurements. The indices of the three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards-----	222	400	440

Structural data. The structure of cesium bromotellurate has not been published, but it is thought to be isostructural with potassium chloroplatinate because of the similarity of patterns. Ewing and Pauling [1] in 1928 determined the structure of potassium chloroplatinate. The NBS pattern is indexed assuming the space group Fm3m (No. 225) with 4(Cs₂TeBr₆) per unit cell.

Lattice constants

1959	National Bureau of Standards-----	A 10.919 at 25° C
------	-----------------------------------	-------------------------

The density of cesium bromotellurate calculated from the NBS lattice constant is 4.452 g/cm³ at 25°C.

Reference

[1] F. J. Ewing and L. Pauling, The crystal structure of potassium chloroplatinate, *Z. Krist.* **68**, 223-230 (1928).

Cesium Bromotellurate, Cs₂TeBr₆ (cubic)

hkl	1959 National Bureau of Standards Cu, 1.5405 Å at 25° C		
	d	I	a
	A		A
111	6.31	27	10.92
200	5.46	4	10.92
220	3.862	37	10.92
311	3.295	17	10.92
222	3.151	100	10.92
400	2.728	86	10.91
331	2.505	6	10.92
420	2.439	4	10.91
422	2.229	16	10.92
511	2.1007	7	10.916
440	1.9301	48	10.918
531	1.8457	6	10.919
620	1.7269	4	10.922
533	1.6656	4	10.922
622	1.6466	24	10.922
444	1.5766	14	10.923
711	1.5294	4	10.922
642	1.4590	6	10.918
731	1.4213	3	10.917
800	1.3649	6	10.919
822	1.2867	2	10.918
662	1.2527	4	10.921
840	1.2209	10	10.920
911	1.1984	2	10.918
664	1.1638	1	10.917
931	1.1449	1	10.922
844	1.1147	5	10.922
933	1.0976	3	10.921
10·2·0	1.0710	2	10.922
951	1.0558	2	10.921
10·2·2	1.0509	3	10.921
953	1.0184	2	10.921
10·4·2	0.9966	3	10.917
11·1·1	.9845	1	10.919
880	.9650	1	10.918
11·3·1	.9540	1	10.919
10·6·0	.9362	1	10.918
10·6·2	.9228	3	10.919
12·0·0	.9098	5	10.918
12·2·2	.8857	2	10.920
12·4·0	.8632	2	10.919
Average value of last five lines-----			10.919

Cesium Nitrate, CsNO₃ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0779	3.15 1.99 1.82	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

X-ray data on ASTM card 4-0575 is for a cubic form of cesium nitrate and was obtained at 170° C. **Additional published patterns.** None.

NBS sample. The sample of cesium nitrate was made from solutions of silver nitrate and cesium bromide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent rubidium; 0.001 to 0.01 percent each of calcium and sodium; and 0.0001 to 0.001 percent each of aluminum, iron, potassium, magnesium, and silicon.

The sample is colorless and optically negative. The indices of refraction are $N_e=1.554$ and $N_o=1.560$.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel.....	112	411, 303	330, 114
National Bureau of Standards.....	112	111	003

Structural data. The most recent work on the structure of cesium nitrate was done by Finbak and Hassel [2] in 1937. They gave the most probable space group as P31m (No. 157) with 9(CsNO₃) per unit cell.

Finbak and Hassel [3] report that a cubic phase is stable above 161° C.

Waldbauer and McCann's unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>a</i>	<i>c</i>
1934	Waldbauer and McCann [4]..	$\overset{A}{10.76}$	$\overset{A}{7.70}$
1959	National Bureau of Standards.....	10.950	7.716 at 25° C

<i>hkl</i>	1938		1959	
	Hanawalt, Rinn, and Frevel		National Bureau of Standards	
	Mo, 0.7107 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	$\overset{A}{4}$		$\overset{A}{4}$	
111	4.46	27	4.467	38
112	3.16	100	3.153	100
202	-----	-----	2.996	4
221	} 2.58	27	2.583	11
003			2.573	38
103	-----	-----	2.483	3
302	-----	-----	2.453	2
222	2.23	23	2.232	21
411	} 1.99	40	1.999	19
303			1.996	26
330	} 1.82	33	1.826	18
114			1.820	22
600	} 1.57	13	1.580	3
224			1.576	6
333	} 1.49	20	1.4880	6
115			1.4852	10
522	} 1.41	17	1.4123	6
414			1.4110	9
441	} 1.34	10	1.3476	1
225			1.3446	5
442	1.28	1	1.2892	2
711	} 1.24	5	1.2397	4
415			1.2361	5
505	} 1.19	12	1.1960	5
306			1.1914	4
444	1.11	1	1.1164	2
633	} 1.08	4	1.0833	6
117			1.0806	4
217	-----	-----	1.0539	2
900	-----	-----	1.0507	2
336	-----	-----	-----	-----
516	-----	-----	1.0265	1
445	-----	-----	1.0242	1
227	-----	-----	1.0220	1

The density of cesium nitrate calculated from the NBS lattice constants is 3.635 g/cm³ at 25° C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
- [2] C. Finbak and O. Hassel, The structure of caesium nitrate, J. Chem. Phys. 5, 460-461 (1937).
- [3] C. Finbak and O. Hassel, Rotation von Anionpolyedern in kubischen Kristallgittern. III. Die Nitrate, Z. physik. Chem. 35, 25-28 (1937).
- [4] L. Waldbauer and D. C. McCann, Caesium nitrate and the perovskite structure, J. Chem. Physics 2, 615-617 (1934).

beta-Chromium Orthophosphate, β -CrPO₄ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
*5-0662	2.48 3.51 4.30	Copper	National Bureau of Standards [1] 1951, [2] 1952.

* This ASTM card was reported without indexing.

Additional published patterns. None.

NBS sample. The sample of beta-chromium orthophosphate was prepared at the NBS by heating the unground hexahydrate between 1,000°C and 1,100°C for $\frac{1}{2}$ hr. Longer heating or heating finely ground hexahydrate tends to produce the stable alpha form. Spectrographic analysis showed no impurities greater than 0.001 percent.

The sample has an olive green color. The very fine highly birefringent particles show no extinction positions and have an average index of 1.908.

Interplanar spacings and intensity measurements. The indices of the three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards-----	112	111	110

Structural data. Mooney [3] in 1956 determined that beta-chromium orthophosphate has the space group Cmc₂m (No. 63) and 4(CrPO₄) per unit cell.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
1956	Mooney [3]-----	<i>A</i> 5.15	<i>A</i> 7.77	<i>A</i> 6.11
1957	Hughes, Lewis and Wilson [4]-----	5.166	7.750	6.131
1959	National Bureau of Standards-----	5.165	7.750	6.131 at 25° C

The density of beta-chromium orthophosphate calculated from the NBS lattice constants is 3.971 g/cm³ at 25° C.

<i>hkl</i>	1959 National Bureau of Standards Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>
	<i>A</i>	
110	4.30	74
020	3.874	41
111	3.520	95
021	3.276	51
200	2.582	50
112	2.497	100
130	2.310	54
220	2.148	5
221	2.030	5
202	1.975	37
040	1.938	20
113	1.845	4
023	1.808	6
222	1.760	28
310	1.681	2
042	1.638	20
311	1.621	5
133	1.533	12
241	1.503	5
150	1.4847	4
312	1.4744	16
114	} 1.4431	7
151		
330	1.4328	10
242	1.3837	37
152	1.3362	6
204	1.3187	6
060	} 1.2917	10
400		
134	1.2778	14
243	1.2351	1
044	} 1.2015	8
421		
115	1.1798	3
333	1.1728	1
350	1.1521	2

References

- [1] Joint Committee Fellowship Report, Nat. Bur. Standards (U.S.), Oct. 1951.
- [2] B. M. Sullivan and H. F. McMurdie, Crystal forms of chromium orthophosphate, *J. Research, Nat. Bur. Standards* **48**, No. 2, 159-162 (1952).
- [3] R. C. L. Mooney, Crystal structure of anhydrous indium phosphate and thallic phosphate by X-ray diffraction, *Acta Cryst.* **9**, 113-117 (1956).
- [4] J. W. Hughes, I. E. Lewis, and A. J. C. Wilson, Comments on the A.S.T.M. X-ray Powder Data File, Cardiff, Great Britain (1957).

Cobalt Aluminum Oxide, CoAl_2O_4 (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-1410	1.43 2.43 1.55	Iron	Natta and Passerini [1] 1929.
3-0896	2.44 2.86 1.43	Molybdenum	Dow Chemical Co.

Additional published patterns

Source	Radiation
Holgersson [2] 1927-----	Iron

NBS sample. The sample of cobalt aluminate was prepared at NBS by solid state reaction by heating hydroxides of cobalt and aluminum at 1,100° C. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium; 0.01 to 0.1 percent each of calcium, iron, magnesium, manganese, nickel, and silicon; 0.001 to 0.01 percent of copper; and 0.0001 to 0.001 percent of chromium.

The color of the sample was deep blue. The index of refraction could not be determined because the sample was too highly colored.

Interplanar spacings and intensity measurements. The d -values reported by Holgersson were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Holgersson-----	511	440	311
Natta and Passerini-----	440	311	511
Dow Chemical Co.-----	311	220	440
National Bureau of Standards-----	311	220	440

Structural data. Holgersson [2] in 1927 determined that cobalt aluminate has the spinel-type structure, the space group $\text{Fd}\bar{3}\text{m}$ (No. 227) and $8(\text{CoAl}_2\text{O}_4)$ per unit cell.

Three unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		A
1927	Holgersson [2]-----	8.09
1929	Natta and Passerini [1]-----	8.08
1934	Krause and Thiel [3]-----	8.09
1959	National Bureau of Standards-----	8.103 at 26° C

hkl	1927 Holgersson Fe, 1.9360 A			1929 Natta and Passerini Fe, 1.9360 A			---- Dow Chemical Co. Mo, 0.7107 A			1959 National Bureau of Standards Cu, 1.5405 A at 26° C		
	d	I	a	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A	A		A
220	2.85	m	8.06	2.86	70	8.09	2.87	50	8.117	2.864	66	8.100
311	2.44	s	8.09	2.43	80	8.06	2.44	100	8.092	2.443	100	8.102
400	-----	----	-----	2.02	60	8.08	2.01	12	8.040	2.026	17	8.104
331	-----	----	-----	-----	----	-----	1.86	2	8.108	1.8608	5	8.111
422	-----	----	-----	1.65	70	8.08	1.65	10	8.083	1.6541	16	8.103
511	1.558	vs	8.10	1.55	80	8.05	1.56	25	8.106	1.5602	34	8.107
440	1.421	vs	8.04	1.428	100	8.09	1.43	50	8.089	1.4324	41	8.103
531	-----	----	-----	1.365	40	8.07	-----	----	-----	1.3716	1	8.114
620	-----	----	-----	1.279	50	8.09	1.27	2	8.032	1.2821	7	8.109
533	-----	----	-----	1.227	50	8.05	1.23	4	8.066	1.2360	2	8.105
642	-----	----	-----	1.078	80	8.07	1.08	4	8.082	1.0826	2	8.101
731	1.051	s	8.07	1.051	80	8.07	1.05	8	8.065	1.0551	3	8.104
800	1.012	s	8.10	1.010	80	8.08	-----	----	-----	1.0131	1	8.105
822	-----	----	-----	-----	----	-----	0.955	2	8.103	0.9547	2	8.101
751	-----	----	-----	-----	----	-----	.936	2	8.105	.9355	2	8.102
Average value of last five lines-----			8.08	-----	----	8.07	-----	----	8.084	-----	----	8.103

28

Structural data. Cobalt oxide has the sodium chloride-type structure, the space group Fm3m (No. 225), and 4(CoO) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		<i>A</i>
1926	Bravo [2]-----	4.33
1928	Natta and Strada [3]-----	4.22
1929	Holgersson and Karlsson [4]-----	4.262
1929	Ingersoll and Hanawalt [5]-----	4.25
1929	Passerini and Natta [6]-----	4.23
1940	Baroni [7]-----	4.23
1950	Tombs and Rooksby [8]-----	4.258
1959	National Bureau of Standards-----	4.260 at 26° C

The density of cobalt oxide calculated from the NBS lattice constant is 6.437 g/cm³ at 26° C.

Cobalt(II,III) Oxide, Co₃O₄ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1-1152	2.43 1.43 1.56	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of cobalt oxide was prepared at NBS by heating cobalt fluoride to 850° C for 24 hr. Spectrographic analysis shows the following impurities: 0.1 to 1.0 percent each of calcium and nickel; 0.01 to 0.1 percent each of aluminum, iron, magnesium, and silicon; and 0.001 to 0.01 percent each of barium, copper, and manganese.

The sample was a black opaque powder.

Interplanar spacings and intensity measurements. The indices of the three strongest lines for each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel-----	311	440	511
National Bureau of Standards-----	311	440	220

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, *Ind. Eng. Chem., Anal. Ed.* **10**, 457-512 (1938).
- [2] F. M. Bravo, Determinacion de la Estructura Cristalina del Oxido de Niquel, del Oxido de Cobalto y del Sulfuro de Plomo, *Anal. Espan. Fis y Quim.* **24**, 611-646 (1926).
- [3] G. Natta and M. Strada, Ossidi ed Ideoossidi del cobalto, *Gazz. Chim. Ital.* **58**, 419 (1928).
- [4] S. Holgersson and A. Karlsson, Roentgenographische Untersuchungen einiger Mischkristallsysteme mit Monoxyden als Komponenten, *Z. Anorg. Chem.* **182**, 255-271, (1929).
- [5] L. R. Ingersoll and J. D. Hanawalt, The gas content, crystal structure and hydrogen absorption of sputtered nickel films, *Phys. Rev.* **34**, 972-977 (1929).
- [6] L. Passarini and G. Natta, Soluzioni Solide Isomorfismo e Simmorfismo tra gli ossidi di metalli bivalenti II, *Gazz. Chim. Ital.* **59**, 144-154 (1929).
- [7] A. Baroni, Sugli Ossidi di Cobalto, *Gazz. Chim. Ital.* **70**, 483 (1940).
- [8] N. C. Tombs and H. P. Rooksby, Structures of monoxide of some transition elements at low temperatures, *Nature* **165**, 442-443 (1950).

<i>hkl</i>	1938			1959		
	Hanawalt, Rinn, and Frevel			National Bureau of Standards		
	Mo, 0.7107 Å			Co, 1.7889 Å at 24° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i> ^a
111	4.68	8	8.11	4.669	22	8.087
220	2.86	20	8.09	2.860	41	8.089
311	2.43	100	8.06	2.438	100	8.085
222	2.34	6	8.11	2.333	11	8.083
400	2.02	13	8.080	2.021	27	8.082
422	1.65	4	8.08	1.6505	11	8.086
511	1.56	25	8.10	1.5559	37	8.085
440	1.43	30	8.09	1.4293	43	8.085
620	-----	-----	-----	1.2788	4	8.088
533	1.24	2	8.13	1.2330	11	8.085
622	-----	---	-----	1.2191	6	8.087
444	-----	---	-----	1.1671	3	8.086
711	-----	---	-----	1.1321	2	8.085
642	1.08	1	8.08	1.0803	6	8.084
731	1.06	4	8.14	1.0524	16	8.084
800	1.01	1	8.08	1.0105	7	8.084
822	-----	---	-----	0.9529	4	8.085
751	0.93	2	8.05	.9335	15	8.084
662	-----	---	-----	.9275	5	8.085
	(^a)					
Average value of last five lines-----			8.10	-----		8.084

^a Two additional lines were omitted.

Structural data. Cobalt oxide is a member of the spinel group, the space group being Fd3m (No. 227) with 8(Co₃O₄) per unit cell [5].

Lattice constants

1928	Hendricks and Albrecht.....	8.06
1928	Natta and Strada.....	8.08
1929	Holgersson and Karlsson.....	8.124
1934	Kraus and Thiel [2].....	8.07
1946	Gulbransen and Hickman.....	8.11
1959	National Bureau of Standards.....	8.084 at 24° C

The density of cobalt oxide calculated from the NBS lattice constants is 6.054 g/cm³ at 24° C.

Dysprosium(III) Oxide, Dy₂O₃ (cubic)

ASTM cards. None.
Additional published patterns

Source	Radiation
Zachariasen [1] 1928.....	Iron

NBS sample. The sample of dysprosium sesquioxide was prepared by the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed the following impurities: a total of less than 0.1 percent of holmium and yttrium oxides and traces of other rare earths. The sample was annealed at 1,100° C for a period of 16 hr.

The sample was colorless. The index of refraction was not determined because the sample was too fine-grained.

Interplanar spacings and intensity measurements. The *d*-values of the Zachariasen pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Zachariasen.....	222	440	622
National Bureau of Standards.....	222	440	400

Structural data. Pauling and Shappell [2] in 1930 determined that dysprosium sesquioxide has the thallium oxide type structure (rare earth type C), the space group Ia3(No. 206) and 16(Dy₂O₃) per unit cell.

The first five unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10**, 451-512 (1938).
- [2] O. Kraus and W. Thiel, Über Keramische Farbkörper, Ber. Deut. Keram. Ges. **15**, 101 (1934).
- [3] E. A. Gulbransen and J. W. Hickman, An electron diffraction study of oxide films formed on iron, cobalt, nickel, chromium, and copper at high temperatures. Metals Technol. **13**, A. I. M. M. E. Tech. Pub. 2068 (1946).
- [4] S. Holgersson and A. Karlsson, Über einige neue Kobaltite vom Spinelltypus. Z. Anorg. Chem. **183**, 384-394 (1929).
- [5] S. B. Hendricks and W. H. Albrecht, X-ray and chemical investigations of various oxides of iron and cobalt, Ber. deut. Keram. Ges. **61B**, 2153-61 (1928).
- [6] G. Natta, M. Strada, Spinelli del cobalto trivalenti: cobaltito cobaltoso e cobaltito di zinco, Rend. Accad. Naz. Lincei **7**, 1024-1030 (1928).

hkl	1928 Zachariasen Fe, 1.9360 Å			1959 National Bureau of Standards Co, 1.7889 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
211	4.37	15	10.69	4.35	15	10.656
222	3.067	100	10.62	3.079	100	10.665
321	2.845	3	10.65	2.850	2	10.664
400	2.655	30	10.62	2.666	42	10.663
411	2.496	8	10.59	2.514	8	10.667
420	-----	---	-----	2.3856	2	10.669
332	2.260	5	10.60	2.2733	6	10.663
422	-----	---	-----	2.1765	1	10.663
431	2.077	15	10.59	2.0911	11	10.663
521	1.931	5	10.58	1.9479	3	10.669
440	1.872	100	10.59	1.8848	44	10.662
433	1.818	5	10.60	1.8288	3	10.664
600	1.760	18	10.56	1.7779	<1	10.667
611	1.718	15	10.59	1.7298	6	10.663
620	1.675	<2	10.59	1.6865	1	10.666
541	1.635	10	10.60	1.6458	5	10.666
622	1.596	100	10.58	1.6079	34	10.666
631	1.561	15	10.59	1.5726	7	10.666
444	1.529	20	10.59	1.5395	8	10.666
543	1.497	10	10.59	1.5087	3	10.668
640	1.468	5	10.58	1.4793	1	10.667
721	1.440	15	10.58	1.4517	4	10.668
642	1.415	10	10.59	1.4255	2	10.667
732	1.345	10	10.59	1.3548	3	10.668
800	1.324	20	10.59	1.3334	5	10.667
811	1.304	25	10.59	1.3131	4	10.667
820	1.285	10	10.50	1.2935	2	10.666
653	1.267	15	10.60	1.2748	3	10.666
822	1.250	10	10.60	1.2570	2	10.666
831	1.233	25	10.61	1.2399	5	10.666
662	1.226	60	10.68	1.2234	10	10.665
840	1.1862	40	10.610	1.1926	8	10.667
833	1.1713	8	10.607	1.1779	1	10.666
842	1.1581	8	10.614	1.1638	2	10.666
921	1.1453	20	10.621	1.1501	3	10.666

hkl	1928 Zachariasen Fe, 1.9360 Å			1958 National Bureau of Standards Co, 1.7889 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
851	1.1187	20	10.613	1.1243	3	10.666
932	-----	---	-----	1.1001	3	10.666
844	-----	---	-----	1.0886	7	10.666
941	-----	---	-----	1.0774	3	10.666
10·0·0	-----	---	-----	1.0666	2	10.666
10·1·1	-----	---	-----	1.0562	1	10.667
10·2·0	-----	---	-----	1.0458	4	10.665
943	-----	---	-----	1.0361	1	10.667
10·2·2	-----	---	-----	1.0264	10	10.667
10·3·1	-----	---	-----	1.0170	4	10.666
871	-----	---	-----	0.9989	5	10.665
10·4·0	-----	---	-----	.9903	4	10.666
10·3·3	-----	---	-----	.9818	3	10.665
10·4·2	-----	---	-----	.9736	4	10.665
954	-----	---	-----	.9656	3	10.665
11·2·1	-----	---	-----	.9501	4	10.665
880	-----	---	-----	.9427	2	10.665
10·4·4	-----	---	-----	.9283	2	10.665
11·3·2	-----	---	-----	.9214	4	10.665
10·6·0	-----	---	-----	.9145	2	10.665
11·4·1	-----	---	-----	.9079	3	10.665
Average value of last five lines--			10.613	-----	---	10.665

		<i>A</i>
1925	Goldschmidt, Barth, and Lunde [3]---	10.65
1928	Zachariasen [1]-----	10.65
1939	Bommer [4]-----	10.650
1954	Templeton and Dauben [5]-----	10.667
1959	National Bureau of Standards-----	10.665 at 25° C

The density of dysprosium sesquioxide calculated from the NBS lattice constant is 8.167 g/cm³ at 25° C.

References

- [1] W. Zachariasen, The crystal structure of the sesquioxides and compounds of the type ABO₃, Skrifter Norske Videnskaps-Akad., Oslo I. Mat.-Naturv. Kl. 1928, No. 4 (1928).
- [2] L. Pauling and M. D. Shappell, The crystal structure of Bixbyite and the C-modification of the sesquioxides, Z. Krist. **75**, 128-142 (1930).
- [3] V. M. Goldschmidt, T. Barth, and G. Lunde, Isomorphie und Polymorphie der Sesquioxide, die Lanthaniden-Kontraktion und ihre Konsequenzen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. 7, 1-59 (1925).
- [4] H. Bommer, Die Gitterkonstanten der C-Formen der Oxyde der seltenen Erdmetalle, Z. anorg. u. allgem. Chem. **241**, 273-280 (1939).
- [5] D. H. Templeton and C. H. Dauben, Lattice parameters of some rare earth compounds and a set of crystal radii, J. Am. Chem. Soc. **76**, 5237-5239 (1954).

Erbium Phosphate, ErPO₄ (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of erbium phosphate was prepared hydrothermally at 400° C from erbium oxide and dilute phosphoric acid. Spectrographic analysis showed no impurities greater than 0.01 percent.

The sample has a pink color. The indices of refraction were not determined because of the small particle size.

Interplanar spacings and intensity measurements. The indices of the three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards-----	200	112	101

Structural data. The structure of erbium phosphate has not been published. It is thought to have a zirconium silicate-type structure because of similarity of patterns. The NBS pattern was indexed assuming the space group to be I4₁/amd (No. 141) with 4(ErPO₄) per unit cell.

Lattice constants

		<i>a</i>	<i>c</i>
		<i>A</i>	<i>A</i>
1959	National Bureau of Standards-----	6.863	6.007 at 25° C

The density of erbium phosphate calculated from the NBS lattice constants is 6.155 g/cm³ at 25° C.

Erbium Phosphate, ErPO₄ (tetragonal)

<i>hkl</i>	1959		<i>hkl</i>	1959	
	National Bureau of Standards			National Bureau of Standards	
	Cu, 1.5405 Å at 25° C			Cu, 1.5405 Å at 25°C	
	<i>d</i>	<i>I</i>		<i>d</i>	<i>I</i>
	<i>A</i>			<i>A</i>	
101	4.52	56	325	1.0161	2
200	3.432	100	631	1.0081	2
211	2.733	23	613	0.9833	5
112	2.554	67	116	.9808	<1
220	2.426	19	415	.9743	1
202	2.261	11	701	.9678	1
301	2.1382	25	640	.9520	3
103	1.9224	14	543	.9451	3
321	1.8144	19	444	.9441	<1
312	1.7596	44	721	.9313	1
400	1.7157	13	712	.9238	6
213	1.6771	9	604	}	6
411	1.6039	5	316		
420	1.5347	10	505		
303	1.5063	2	624	.8797	5
004	1.5023	4	525	.8745	2
332	1.4244	12	732	.8631	5
323	1.3792	10	800	.8579	2
204	1.3759	<1	723	.8529	2
431	1.3379	6	107	.8514	1
413	1.2802	10	811	.8429	<1
224	1.2769	<1	426	.8380	1
521	1.2465	1	820	.8324	1
512	1.2283	9	217	.8267	1
440	1.2120	2	802	.8225	1
105	1.1832	2	660	.8089	1
600	1.1438	5	644	.8040	8
503	1.1321	<1	307	}	<1
404	1.1301	6	516		
215	1.1189	4	545		
611	1.1089	2	831	.7962	<1
532	1.0957	8	813	.7833	<1
620	1.0851	4	327	.7823	<1
424	1.0732	9			
541	1.0550	1			

Holmium(III) Oxide, Ho₂O₃ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of holmium sesquioxide was prepared by the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed the following impurities: a total of less than 0.1 percent of erbium and dysprosium oxides and traces of other rare earths. The sample was annealed at 1,100° C for a period of 16 hr.

The sample was colorless. The index of refraction was not determined because the sample was too fine-grained.

Interplanar spacings and intensity measurements. The indices of the three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards-----	222	440	400

▀ **Structural data.** Pauling and Shappell [3] in 1930 determined that holmium sesquioxide has the thalliumoxide type structure (rare earth type C), the space group Ia3(No. 206) and 16(Ho₂O₃) per unit cell.

The first three unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Holmium(III) Oxide, Ho₂O₃ (cubic)

<i>hkl</i>	1959			<i>hkl</i>	1959		
	National Bureau of Standards				National Brueau of Standards		
	Co, 1.7889 Å at 25° C				Co, 1.7889 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>		<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>		<i>A</i>		<i>A</i>
211	4.334	14	10.616	662	1.2171	8	10.610
222	3.061	100	10.604	840	1.1861	7	10.609
321	2.835	2	10.608	833	1.1715	1	10.608
400	2.651	41	10.606	842	1.1576	1	10.610
411	2.500	7	10.606	921	1.1440	3	10.609
420	2.3723	1	10.609				
332	2.2613	5	10.606	851	1.1182	2	10.608
422	2.1652	1	10.607	932	1.0942	3	10.609
431	2.0796	10	10.604	844	1.0827	6	10.608
521	1.9361	3	10.604	941	1.0715	2	10.607
				10·0·0	1.0608	2	10.608
440	1.8754	42	10.609				
433	1.8195	3	10.609	10·1·1	1.0504	1	10.608
600	1.7670	<1	10.602	10·2·0	1.0400	4	10.606
611	1.7204	6	10.605	943	1.0302	1	10.607
620	1.6767	1	10.604	10·2·2	1.0206	7	10.606
541	1.6366	5	10.606	10·3·1	1.0112	4	10.606
622	1.5989	30	10.606				
631	1.5637	7	10.606	871	0.9934	3	10.606
444	1.5311	7	10.608	10·4·0	.9848	4	10.607
543	1.4997	2	10.604	10·3·3	.9764	2	10.607
				10·4·2	.9682	4	10.606
640	1.4706	1	10.605	954	.9603	3	10.607
721	1.4434	3	10.607				
642	1.4170	2	10.604	11·2·1	.94491	4	10.6066
732	1.3468	3	10.605	880	.93744	2	10.6059
800	1.3259	4	10.607	10·4·4	.92317	2	10.6064
				11·3·2	.91625	4	10.6064
811	1.3056	4	10.607	10·6·0	.90949	2	10.6064
820	1.2863	2	10.607				
653	1.2680	3	10.609	Average value of last five lines ---			10.6063
822	1.2503	1	10.609				
831	1.2333	4	10.609				

Lattice constants

		<i>A</i>
1925	Goldschmidt, Barth, and Lunde [2]---	10.60
1927	Zachariasen [1]-----	10.60
1954	Templeton and Dauben [4]-----	10.607
1959	National Bureau of Standards-----	10.606 at 25° C

The density of holmium sesquioxide calculated from the NBS lattice constant is 8.413 g/cm³ at 25° C.

References

- [1] W. Zachariasen, The crystal structure of the modification C of the sesquioxides of the rare earth metals, and of indium and thallium, Norsk. Geol. Tidsskr. 9, 310-316 (1927).
- [2] V. M. Goldschmidt, T. Barth, and G. Lunde, Isomorphie und Polymorphie der Sesquioxide, die Lanthaniden-Kontraktion und ihre Konsequenzen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. 7, 1-59 (1925).
- [3] L. Pauling and M. D. Shappell, The crystal structure of Bixbyite and the C-modification of the sesquioxides, Z. Krist. 75, 128-142 (1930).
- [4] D. H. Templeton and C. H. Dauben, Lattice parameters of some rare earth compounds and a set of crystal radii, J. Am. Chem. Soc. 76, 5237-5239 (1954).

Magnesium Chromite (picrochromite) MgCr_2O_4 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2-1228	2.08 1.60 1.47	Chromium	Holgersson [1] 1930.

Additional published patterns

Source	Radiation
Passerini and Bruni [2] 1929----- Andrews [6] 1951-----	Iron Cobalt

NBS sample. The sample of magnesium chromite was prepared at the NBS by fusion of MgO and Cr_2O_3 in a carbon arc with subsequent heating to

remove carbides. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium and silicon; 0.01 to 0.1 percent of aluminum, calcium, and iron; and 0.001 to 0.01 percent of copper, nickel, strontium, and titanium.

The color of the sample was dark brownish-green. The index of refraction was too high to be measured by the usual oil immersion method.

Interplanar spacings and intensity measurements. Several patterns were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Passerini and Bruni-----	440	400	444
Holgersson-----	400	511	440
Andrews-----	440	840	311
National Bureau of Standards-----	311	111	400

<i>hkl</i>	1929 Passerini and Bruni Fe, 1.9373 A			1930 Holgersson Cr, 2.2909 A			1951 Andrews Co, 1.790 A			1959 National Bureau of Standards Cu, 1.5405 A at 26° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
111	-----	-----	-----	-----	-----	-----	4.81	vvw	8.331	4.813	65	8.335
220	2.863	2	8.10	2.942	20	8.321	2.946	vw	8.333	2.945	13	8.331
311	2.449	17	8.12	2.514	80	8.338	2.512	ms	8.331	2.512	100	8.331
222	2.343	1	8.12	-----	-----	-----	2.406	vw	8.335	2.406	12	8.335
400	2.040	42	8.16	2.083	100	8.332	2.083	ms	8.332	2.083	56	8.332
331	-----	-----	-----	-----	-----	-----	1.912	vvw	8.334	1.912	5	8.334
422	1.676	3	8.21	-----	-----	-----	1.701	vw	8.333	1.701	2	8.333
511	1.589	11	8.26	1.603	100	8.329	1.604	m	8.334	1.603	39	8.332
440	1.463	100	8.28	1.474	100	8.338	1.4731	s	8.333	1.4731	53	8.333
531	1.404	4	8.31	-----	-----	-----	1.4085	vw	8.333	1.4089	13	8.335
620	1.315	2	8.32	1.319	20	8.342	1.3177	vvw	8.334	1.3176	1	8.333
533	1.270	9	8.33	1.273	100	8.348	1.2709	mw	8.334	1.2711	13	8.335
622	1.254	2	8.32	-----	-----	-----	1.2563	mw	8.333	1.2563	9	8.333
444	1.200	33	8.31	-----	-----	-----	1.2028	mw	8.333	1.2028	9	8.333
711	-----	-----	-----	-----	-----	-----	1.1668	w	8.333	1.1666	8	8.331
642	-----	-----	-----	-----	-----	-----	1.1135	vw	8.333	1.0136	2	8.333
731	-----	-----	-----	-----	-----	-----	1.0849	ms	8.333	1.0850	10	8.334
800	-----	-----	-----	-----	-----	-----	1.0417	mw	8.334	1.0417	4	8.334
822	-----	-----	-----	-----	-----	-----	0.9821	vvw	8.333	0.9821	<1	8.333
751	-----	-----	-----	-----	-----	-----	.9622	ms	8.333	.9623	6	8.334
662	-----	-----	-----	-----	-----	-----	.9559	mw	8.333	.9559	1	8.333
840	-----	-----	-----	-----	-----	-----	.9317	s	8.333	.9317	6	8.333
911	-----	-----	-----	-----	-----	-----	.9147	ms	8.333	.9146	4	8.332
931	-----	-----	-----	-----	-----	-----	-----	-----	-----	.8736	5	8.333
844	-----	-----	-----	-----	-----	-----	-----	-----	-----	.8505	9	8.333
933	-----	-----	-----	-----	-----	-----	-----	-----	-----	.8375	2	8.333
951	-----	-----	-----	-----	-----	-----	-----	-----	-----	.8056	8	8.333
10·2·2	-----	-----	-----	-----	-----	-----	-----	-----	-----	.8019	3	8.334
Average value of last five lines-----	8.32	-----	-----	8.338	-----	-----	-----	-----	8.333	-----	-----	8.333

Structural data. Passerini and Bruni [2] in 1929 showed that magnesium chromite has the spinel-type structure, the space group Fd3m (No. 227) and 8(MgCr₂O₄) per unit cell.

The first five unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>A</i>
1929	Passerini and Bruni [2]-----	8.31
1930	Holgersson [1]-----	8.34
1946	Lovell, Rigby, and Green [3]-----	8.33
1946	Rait [4]-----	8.325
1946	Verwey, Haayman, and Heilman [5]---	8.33
1951	Andrews [6]-----	8.323
1959	National Bureau of Standards-----	8.333 at 26° C

Manganese Aluminate (galaxite), MnAl₂O₄ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1-1302	1.40 2.50 2.39	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Holgersson [2] 1927-----	Iron Molybdenum
Clark, Ally, and Badger [3] 1931-----	

NBS sample. The sample of manganese aluminate was made at NBS by heating MnCO₃ and Al(OH)₃ to 1,300° C for 24 hr. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of cobalt and sodium; 0.01 to 0.1 percent silicon; and 0.001 to 0.01 percent each of chromium, copper, iron, and magnesium.

The color of the sample was brown. The index of refraction could not be determined because the sample was too dark.

Interplanar spacings and intensity measurements. The *d*-values reported by Clark, Ally, and Badger [3] were modified to correspond to a wavelength change of K_{α1} 0.712 to K_{α1} 0.7093 Å. The *d*-values reported by Holgersson [2] and Hanawalt, Rinn, and Frevel [1] were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

The density of magnesium chromite calculated from the NBS lattice constant is 4.414 g/cm³ at 26° C.

References

- [1] S. Holgersson, Röntgenographische Untersuchungen einiger synthetisch dargestellten Chromspinelle, *Z. anorg. Chem.* **192**, 123-128 (1930).
- [2] L. Passerini and S. Bruni, Ricerche Sugli Spinelli, *Rend. Accad. Naz. Lincei* **9**, 338-343 (1929).
- [3] G. H. B. Lovell, G. R. Rigby, and A. T. Green, An investigation of chrome ores, *Iron and Steel Inst. Spec. Report* **32**, 153-170 (1946).
- [4] J. R. Rait, An X-ray investigation into the constitution of chrome ores, *Iron and Steel Spec. Report* **32**, 175-209 (1946).
- [5] E. J. W. Verwey, P. W. Haayman, and E. L. Heilman, On the crystalline structure of ferrites and analogous metal oxides, *Philips Tech. Rev.* **9**, 185-190 (1946).
- [6] K. W. Andrews, An X-ray study of spinels in relation to chrome magnesite refractories, *Trans. Brit. Ceram. Soc.* **50**, 47-74 (1951).

Pattern	1	2	3
Hanawalt, Rinn, and Frevel-----	---	311	222
Holgersson-----	311	400	511
Clark, Ally, and Badger-----	311	220	511
National Bureau of Standards-----	311	220	440

Structural data. Bragg [4] in 1915 determined the structure of the spinel group. Manganese aluminate has the spinel-type structure, the space group Fd3m (No. 227), and 8(MnAl₂O₄) per unit cell.

Several published unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>A</i>
1927	Holgersson [2]-----	8.28
1931	Clark, Ally, and Badger [3]-----	8.24
1931	Krause and Thiel [5]-----	8.29
1959	National Bureau of Standards-----	8.258 at 25° C

The density of manganese aluminate calculated from the NBS lattice constant is 4.077 g/cm³ at 25° C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, *Ind. Eng. Chem., Anal. Ed.* **10**, 451-512 (1938).
- [2] S. Holgersson, X-ray examination of the minerals of the spinel group and of synthesized substances of the spinel type, *Lunds Univ. Årsskr.* **23**, No. 9, 1-112 (1927).
- [3] G. L. Clark, A. Ally, and A. E. Badger, The lattice dimensions of spinels, *Am. J. Sci.* **22**, 539-546 (1931).
- [4] W. H. Bragg, The structure of the spinel group of crystals, *Nature* **95**, 561 (1915).
- [5] O. Krause and W. Thiel, The structure of some ceramic coloring materials containing aluminum oxide, *Z. Anorg. Chem.* **203**, 120-128 (1931).

Manganese Aluminate (galaxite), MnAl_2O_4 (cubic)

<i>hkl</i>	1938			1927			1931			1959		
	Hanawalt, Rinn, and Frevel			Holgersson			Clark, Ally, and Badger			National Bureau of Standards		
	Mo, 0.7107 Å			Fe, 1.9373 Å			Mo, 0.7093 Å			Cu, 1.5405 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
220	2.93	17	8.29	2.921	w	8.26	2.91	70	8.231	2.921	58	8.262
311	2.50	50	8.29	2.499	vs	8.29	2.48	100	8.225	2.494	100	8.265
222	2.39	50	8.28	-----	-----	-----	2.38	5	8.245	2.383	10	8.254
400	-----	-----	-----	2.073	vs	8.29	2.057	20	8.228	2.065	21	8.260
422	-----	-----	-----	-----	-----	-----	1.678	20	8.220	1.6862	19	8.260
511	-----	-----	-----	1.588	vs	8.25	1.590	70	8.262	1.5896	41	8.262
440	-----	-----	-----	1.461	vs	8.262	1.460	70	8.259	1.4600	44	8.259
-----	1.401	100	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
620	-----	-----	-----	-----	-----	-----	1.300	5	8.222	1.3060	7	8.260
533	-----	-----	-----	1.261	vw	8.272	1.259	10	8.256	1.2596	11	8.262
642	-----	-----	-----	-----	-----	-----	1.101	10	8.239	1.1037	9	8.262
731	-----	-----	-----	1.075	s	8.256	1.075	20	8.257	1.0749	22	8.257
800	-----	-----	-----	-----	-----	-----	1.032	10	8.256	1.0322	12	8.256
822	-----	-----	-----	-----	-----	-----	0.970	20	8.231	0.9732	7	8.258
751	-----	-----	-----	-----	-----	-----	.951	20	8.236	.9534	19	8.257
931	-----	-----	-----	-----	-----	-----	.866	10	8.261	.8656	16	8.257
844	-----	-----	-----	-----	-----	-----	.842	10	8.250	.8429	27	8.259
10·2·0	-----	-----	-----	-----	-----	-----	.809	5	8.250	.8097	11	8.257
951	-----	-----	-----	-----	-----	-----	.798	10	8.255	.7983	17	8.258
Average value of last five lines-----			8.29	-----	-----	8.266	-----	-----	8.250	-----	-----	8.258

Manganese Ferrite (jacobsite), MnFe_2O_4 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
8-15	2.56 2.12 1.64	Iron	McAndrew [1] 1952.

Additional published patterns

Source	Radiation
Holgersson [2] 1927-----	Iron Iron
Passerini [3] 1930-----	

of aluminum and silicon; and 0.001 to 0.01 percent each of chromium, copper, calcium, magnesium, molybdenum, and nickel.

The sample was a blackish opaque powder.

Interplanar spacings and intensity measurements.

The pattern reported by Passerini was converted from kX to angstrom units. The *d*-values for the Holgersson pattern were calculated from Bragg angle data. The indices for the three strongest lines for each pattern are as follows:

Pattern	1	2	3
McAndrew-----	311	400	511
Holgersson-----	311	400	731
Passerini-----	440	800	311
National Bureau of Standards-----	311	440	220

NBS sample. The sample of jacobsite was prepared at NBS by solid state reaction at approximately 1,100° C between Fe_2O_3 and MnCO_3 using KCl as a flux. The KCl was washed out after the reaction was completed. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of titanium and zinc; 0.01 to 0.1 percent each

Structural data. Bragg [4] in 1915 described the structure of the spinel group. Jacobsite has the spinel-type structure, the space group $\text{Fd}\bar{3}\text{m}$ (No. 227), and $8(\text{MnFe}_2\text{O}_4)$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Manganese Ferrite (jacobsite), MnFe_2O_4 (cubic)

<i>hkl</i>	1952 McAndrew			1927 Holgersson			1930 Passerini			1959 National Bureau of Standards		
	Fe, 1.9373 Å			Fe, 1.9373 Å			Fe, 1.9373 Å			Fe, 1.93597 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
111	4.94	40	8.56	-----	----	-----	-----	----	-----	4.906	21	8.497
220	3.01	40	8.51	3.03	w	8.57	2.97	9	8.41	3.005	37	8.500
311	2.56	100	8.49	2.59	vs	8.59	2.54	30	8.43	2.563	100	8.501
222	2.45	3	8.49	-----	----	-----	-----	----	-----	2.450	11	8.487
400	2.12	60	8.48	2.16	vs	8.64	2.11	24	8.44	2.124	26	8.495
422	1.739	10	8.56	-----	----	-----	1.73	10	8.46	1.7342	20	8.496
511	1.636	60	8.50	1.66	s	8.63	1.631	18	8.48	1.6355	34	8.498
440	1.501	60	8.49	1.46	vw	8.64	1.500	100	8.48	1.5031	42	8.503
531	1.435	5	8.49	-----	----	-----	1.437	3	8.50	1.4376	2	8.505
620	1.339	3	8.47	-----	----	-----	1.346	8	8.51	1.3441	3	8.501
533	1.296	20	8.50	1.309	w	8.58	1.300	14	8.52	1.2962	21	8.500
622	1.278	5	8.48	-----	----	-----	1.284	5	8.52	1.2810	14	8.497
444	1.225	10	8.49	1.233	vw	8.54	1.230	18	8.52	1.2276	8	8.505
711	1.191	3	8.50	-----	----	-----	1.194	1	8.53	1.1898	10	8.497
642	1.134	5	8.49	1.148	w	8.59	1.139	13	8.52	1.1355	7	8.501
731	1.108	40	8.51	1.114	vs	8.56	1.112	24	8.54	1.1063	28	8.498
800	1.062	20	8.50	1.071	s	8.57	1.067	35	8.54	1.0623	12	8.498
751	0.982	40D	8.50	-----	----	-----	-----	----	-----	0.9815	21	8.500
Average value of last five lines-----			8.50	-----	----	8.57	-----	----	8.53	-----	----	8.499

Lattice constants

		<i>A</i>
1927	Holgersson [2]-----	8.572
1930	Passerini [3]-----	8.532
1934	Krause and Thiel [5]-----	8.597
1952	McAndrew [1]-----	8.505
1959	National Bureau of Standards-----	8.499 at 25° C

References

- [1] J. McAndrew, The cell edge of jacobsite, *Am. Min.* **37**, 453-460 (1952).
- [2] S. Holgersson, Röntgenographische Untersuchungen der Spinelle, *Acta Univ. Lundensis* **23**, 22-112 (1927).
- [3] L. Passerini, Ricerche sugli spinelli, *Gazz. chim. itali.* **60**, 389-399 (1930).
- [4] W. H. Bragg, The structure of magnetite and the spinels, *Nature* **95**, 561 (1915).
- [5] O. Krause and W. Thiel, Ueber keramische Farbkörper, *Ber. deut. keram. Ges.* **15**, 101-110 (1934).

The density of jacobsite, calculated from the NBS lattice constant, is 4.989 g/cm³ at 25° C.

Manganese(III) Oxide (partridgeite), Mn_2O_3 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2-0896	2.72 1.66 1.42	Iron	Zachariasen [1] 1928.

Additional published patterns

Source	Radiation
Drucker and Hüttner [2] 1928-----	Iron Chromium Iron
Wretblad [3] 1930-----	
Morozov and Kuznecov [4] 1949-----	

Manganese(III) Oxide, (partridgeite) Mn_2O_3 (cubic)

	1928			1928			1930			1949			1959		
	Zachariasen Fe, 1.9373 Å			Drucker and Huttner Fe, 1.9373 Å			Wrethblad Cr, 2.2909 Å			Morozov and Kuznetsov Fe, 1.9373 Å			National Bureau of Standards Fe, 1.93597 Å at 25° C		
	<i>a</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
<i>hkl</i>															
200	A		A	A			A		A	A		A	A		A
211	3.86	15	9.46	3.75	vw		3.84	s	9.40	3.84	44	9.42	4.70	2	9.41
							3.33	vw					3.84	23	9.41
							2.98	s							
222	2.72	100	9.43	2.70	s		2.72	vs	9.41	2.73	100	9.46	2.72	100	9.41
321							2.52	m	9.41	2.54	22	9.50	2.51	3	9.40
400	2.35	10	9.42	2.34	w		2.35	s	9.42	2.35	44	9.42	2.35	11	9.41
411							2.22	vw	9.40				2.22	<1	9.40
420							2.10	w	9.40				2.10	1	9.40
332	2.01	20	9.42	1.99	m		2.01	s	9.40	2.01	56	9.41	2.01	13	9.41
422							1.919	m	9.40	1.931	11	9.46	1.920	<1	9.40
431	1.842	30	9.39	1.836	m		1.845	s	9.41	1.850	67	9.43	1.845	13	9.41
521				1.710	vw		1.717		9.40	1.724	22	9.42	1.719	3	9.42
440	1.663	90	9.41	1.656	s		1.663	vs	9.41	1.664	89	9.42	1.664	32	9.41
433							1.614	m	9.41	1.614	11	9.40	1.615	1	9.42
600							1.567	w	9.40	1.563	11	9.39	1.563	<1	9.39
611				1.524	vw		1.525	m	9.40	1.530	33	9.43	1.527	4	9.41
620							1.487	w	9.40	1.489	22	9.42	1.487	1	9.40
541	1.453	20	9.42	1.449	m		1.4514	s	9.406	1.454	44	9.42	1.4524	8	9.413
622	1.419	60	9.41	1.414	s		1.4183	vs	9.408	1.421	67	9.43	1.4191	15	9.413
631	1.387	20	9.41	1.384	m		1.3873	m	9.409	1.388	44	9.41	1.3875	5	9.410
444	1.356	15	9.39	1.352	w		1.3583	m	9.411	1.361	33	9.43	1.3589	2	9.415
							1.3306	w		1.325	11				
640				1.302	vw		1.3044	m	9.406	1.304	22	9.40	1.3053	2	9.413
721	1.282	15	9.42	1.276	w		1.2802	m	9.408	1.285	44	9.42	1.2801	4	9.407
642				1.254	vw		1.2577	w	9.412	1.267	11	9.48	1.2583	2	9.416
				1.233	vw		1.2355	w							
732	1.195	5	9.41	1.189	w		1.1950	s	9.409	1.193	22	9.40	1.1949	2	9.409
800	1.177	15	9.42	1.174	w		1.1766	s	9.413	1.177	44	9.418	1.1764	2	9.411
811	1.159	15	9.42	1.153	w		1.1585	s	9.412	1.159	56	9.419	1.1582	3	9.409
821	1.144	15	9.43							1.141	44	9.413	1.1418	2	9.416
653				1.121	vw					1.124	44	9.410	1.1251	1	9.413
822				1.104	vw					1.111	11	9.420	1.1089	<1	9.409
831										1.094	11	9.416	1.0936	2	9.408
662				1.076	vw					1.080	56	9.416	1.0793	4	9.409
Average value of last five lines.			9.42						9.411		(^a)				9.411

^a Four additional lines were omitted.

NBS sample. The sample of manganese sesquioxide was prepared at NBS by heating specially purified manganese dioxide contributed by Malinckrodt Chemical Works at 850° C for 16 hr. Their spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of potassium and sodium; and 0.001 to 0.01 percent each of copper, lead, and molybdenum.

The sample was an opaque black powder.

Interplanar spacings and intensity measurements. The *d*-values reported by Morozov and Kuznecov were converted from kX to angstrom units and the *d*-values reported by Zachariasen, Drucker and Hüttner, and Wretblad were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Zachariasen.....	222	440	622
Drucker and Hüttner.....	222	440	622
Wretblad.....	222	440	622
Morozov and Kuznecov.....	222	440	431
National Bureau of Standards.....	222	440	211

Structural data. Pauling and Shappell [5] in 1930 determined that manganese sesquioxide has the thallium oxide-type structure, the space group Ia3 No. 206) and 16(Mn₂O₃) per unit cell.

Mercury(II) Oxide (montroydite), HgO (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
5-0596	2.97 2.83 2.41	Copper	National Bureau of Standards [1] 1954.

The pattern reported on ASTM card No. 5-0596 has been reindexed to conform with the new cell size. The indexing on this card was based upon the unit cell and space group Pmmn proposed by Zachariasen [2]. More recent work by Aurivillius [3] with neutron diffraction indicates the "a" should be doubled and the space group should be Pnma. Eight lines of weak intensity have also been added.

Interplanar spacings and intensity measurements. The indices of the three strongest lines of the NBS pattern are as follows:

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>A</i>
1928	Zachariasen [1].....	9.43
1930	Wretblad [3].....	9.410
1949	Morozov and Kuznecov [4].....	9.42
1959	National Bureau of Standards.....	9.411 at 25° C

The density of manganese sesquioxide calculated from the NBS lattice constants is 5.031 g/cm³ at 25° C.

References

- [1] W. H. Zachariasen, On the crystal structure of bixbyite and artificial Mn₂O₃, *Z. Krist.* **67**, 455-464 (1928).
- [2] D. Drucker and R. Hüttner, Die Thermische Dissoziation des Mangandioxydes, *Z. physik. Chem.* **131**, 237-266 (1928).
- [3] P. E. Wretblad, Röntgenographische Untersuchung der Systeme Fe₂O₃-Cr₂O₃ und Fe₂O₃-Mn₂O₃, *Z. anorg. u. allgem. Chem.* **189**, 329-336 (1930).
- [4] I. S. Morozov and V. G. Kuznecov, The γ modification of manganese dioxide, *Izvest. Akad. Nauk. SSSR Otdel. Khim. Nauk.* #4, 343-353 (1949).
- [5] L. Pauling and M. D. Shappell, The crystal structure of bixbyite and the C-modification of the sesquioxides, *Z. Krist.* **75**, 128-142 (1930).

Pattern	1	2	3
National Bureau of Standards.....	011	210	201

Structural data. Aurivillius [3] in 1956 determined that mercuric oxide has the space group Pnma (No. 62) and 4(HgO) per unit cell. The new unit-cell measurements are compared with the previous measurements reported.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		<i>A</i>	<i>A</i>	<i>A</i>
1954	National Bureau of Standards [1].....	3.304	5.518	3.519
1956	Aurivillius [3].....	6.612	5.520	3.521
1959	National Bureau of Standards.....	6.608	5.518	3.519 at 25° C

Mercury (II) Oxide (montroydite), HgO
(orthorhombic)

The density of mercuric oxide calculated from the NBS lattice constants is 11.209 g/cm³ at 25° C.

<i>hkl</i>	1959	
	National Bureau of Standards	
	Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>
	Å	
200	3.302	1
101	3.101	2
011	2.967	100
210	2.834	81
020	2.759	58
201	2.408	67
211	2.206	2
220	2.117	<1
121	2.062	<1
221	1.814	49
002	*1.759	11
400	1.651	11
031	1.630	15
230	1.607	13
131	} 1.583	2
410		
321	1.547	1
401	} 1.495	25
212		
022	1.484	12
411	1.443	18
420	1.417	11
040	1.379	4
421	1.315	1
402	1.204	5
241	1.1971	10
232	1.1866	9
431	1.1605	7
013	1.1475	4
203	1.1052	6
422	1.1039	8
042	1.0855	3
610	1.0801	3
440	1.0589	4
051	1.0532	4
601	1.0510	4
531	} 1.0262	5
223		
033	0.9890	3
621	.9823	4
630	.9450	5
413	.9425	3
612	.9202	4
442	.9072	3
252	} .8996	4
711		

References

- [1] National Bureau of Standards, Standard X-ray diffraction powder patterns, Nat. Bur. Standards Circ. 539 **III**, 35-37 (1954).
- [2] W. Zachariasen, Über die Kristallstruktur des Quecksilberoxyds, Z. physik. Chem. **128**, 421-429 (1927).
- [3] K. Aurivillius, The crystal structure of mercury(II) Acta Cryst. **9**, 685-686 (1956).

Neodymium Ethylsulfate Nonahydrate, $\text{Nd}[(\text{C}_2\text{H}_5)\text{SO}_4]_3 \cdot 9\text{H}_2\text{O}$ (hexagonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of neodymium ethylsulfate nonahydrate was prepared at NBS by E. L. Weise. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent magnesium; and 0.001 to 0.01 percent each of calcium, sodium, and silicon.

The color of the sample was light purple and it was optically positive. The indices of refraction are $N_o = 1.478$ and $N_e = 1.484$.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards.....	201	211	111

Structural data. Ketelaar [1] in 1937 determined that neodymium ethylsulfate nonahydrate has the space group $P6_3/m$ (No. 176) with $2\{\text{Nd}[(\text{C}_2\text{H}_5)\text{SO}_4]_3 \cdot 9\text{H}_2\text{O}\}$ per unit cell.

The unit-cell measurements reported by Ketelaar have been converted from kX to angstrom units for comparison with the NBS values.

hkl	1959		hkl	1959	
	National Bureau of Standards			National Bureau of Standards	
	Cu, 1.5405 Å at 25° C			Cu, 1.5405 Å at 25° C	
	d	I		d	I
	A				
100	12.17	56	332	1.954	19
110	7.02	18	601	1.945	15
101	6.14	76	520		
200	6.07	76			
111	5.00	90	313	1.940	19
			422	1.929	10
201	4.620	100	431	1.925	10
300	4.055	68	403	1.869	10
211	3.858	93	512	1.8606	10
002	3.556	32			
301	3.517	24	610	1.8524	15
			323	1.8064	14
310	3.372	25	611	1.7931	12
112	3.174	7	004	1.7797	8
221	3.146	26	104	1.7602	8
202	3.072	15			
311	3.047	20	432	1.7418	6
			700	1.7360	7
400	3.037	19	114	1.7238	5
212	2.813	50	204	1.7069	10
320	2.788	50	522		
302	2.673	28			
410	2.652	26	503	1.6972	10
			701	1.6857	12
321	2.595	38	423	1.6493	10
222	2.499	15	612	1.6428	12
312	2.447	11	621	1.6396	13
500	2.430	11			
330	2.339	16	304	1.6294	7
			710	1.6093	21
103	2.329	12	513	1.6058	18
402	2.310	8	224	1.5860	6
501	2.298	41	314	1.5729	10
420			442		
322					
	2.195	32			
421	2.185	39	702	1.5596	5
510			630	1.5312	7
412			433	1.5276	7
213	2.127	47	622	1.5219	10
511	2.108	24	541	1.5194	12
	2.087	39			
600	2.026	14	324	1.5002	6
502	2.008	5	631	1.4962	8
430	1.998	10	801	1.4852	5
			414	1.4775	7

The density of neodymium ethylsulfate nonahydrate calculated from the NBS lattice constants is 1.867 g/cm³ at 25° C.

References

[1] J. A. A. Ketelaar, The crystal structure of the ethylsulfates of the rare earths and yttrium, *Physica* 4, 619-630 (1937).

Nickel Aluminate, NiAl₂O₄ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1-1299	1.42 2.43 2.01	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Holgersson [2] 1927.....	Iron

NBS sample. The sample of nickel aluminate was prepared at NBS by heating co-precipitated

hydroxides at 1,300°C. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium; 0.01 to 0.1 percent each of cobalt and silicon; 0.001 to 0.01 percent each of chromium, iron, and magnesium; and 0.0001 to 0.001 percent each of calcium and manganese.

The sample had a blue color. The index of refraction was 1.825.

Interplanar spacings and intensity measurements.

The *d*-values for the Holgersson pattern were calculated from reported Bragg angle data. The *d*-values for the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units. The three strongest lines for each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel.....	440	311	400
Holgersson.....	311	400	511
National Bureau of Standards.....	311	400	440

<i>hkl</i>	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 Å			1927 Holgersson Fe, 1.9360 Å			1959 National Bureau of Standards Cu, 1.5405 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
111	-----	-----	-----	-----	-----	-----	4.650	22	8.053
220	-----	-----	-----	-----	-----	-----	2.846	22	8.049
311	2.43	75	8.06	2.43	s	8.06	2.427	100	8.049
400	2.01	75	8.04	2.016	s	8.06	2.013	63	8.051
422	-----	-----	-----	1.642	w	8.04	1.6415	7	8.042
511	1.55	13	8.05	1.554	s	8.08	1.5485	29	8.046
440	1.423	100	8.05	1.422	s	8.04	1.4232	60	8.051
531	-----	-----	-----	-----	-----	-----	1.3601	<1	8.046
620	-----	-----	-----	-----	-----	-----	1.2739	<1	8.057
533	-----	-----	-----	1.226	w	8.04	1.2274	8	8.049
622	-----	-----	-----	-----	-----	-----	1.2134	<1	8.049
444	-----	-----	-----	1.159	w	8.03	1.1613	6	8.046
642	-----	-----	-----	1.074	vw	8.04	1.0753	2	8.047
731	-----	-----	-----	1.046	s	8.03	1.0476	11	8.047
800	-----	-----	-----	1.005	w	8.04	1.0061	7	8.049
751	-----	-----	-----	-----	-----	-----	0.9291	7	8.046
840	-----	-----	-----	-----	-----	-----	.8998	6	8.048
844	-----	-----	-----	-----	-----	-----	.8214	15	8.048
Average value of last five lines..			8.05	-----	-----	8.04	-----	-----	8.048

Structural data. Bragg [3] in 1915 determined the structure of the spinel group. Nickel aluminate has the spinel-type structure, the space group $Fd3m$ (No. 227), and $8(\text{NiAl}_2\text{O}_4)$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		<i>A</i>
1927	Holgersson [2].....	8.045
1934	Krause and Thiel [4].....	8.07
1943	Vegard and Borlaug [5].....	8.050
1959	National Bureau of Standards.....	8.048 at 25° C

The density of nickel aluminate, calculated from the NBS lattice constant is 4.501 g/cm^3 at 25°C .

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, *Ind. Eng. Chem., Anal. Ed.* **10**, 457-512 (1938).
- [2] S. Holgersson, Röntgenographische Untersuchung der Mineralien des Spinellgruppe, *Acta Univ. Lundensis* **23**, (1927).
- [3] W. H. Bragg, The structure of magnetite and the spinels, *Nature* **95**, 561 (1915).
- [4] O. Krause and W. Thiel, Ueber Keramischer Farbkörper, *Ber. deut. keram. Ges.* **15**, 100-110 (1934).
- [5] L. Vegard and A. Borlaug, Röntgenstrallanalyse von mischkristallen innerhalb der spinellgruppe, *Avhandl. Norske Videnskaps-Akad. Oslo, I. Mat. Naturv. Kl.* **5**, 1-19 (1943).

Nickel Germinate, Ni_2GeO_4 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of nickel germanate was prepared at NBS by solid state reaction between nickel oxide and germanium oxide at $1,100^\circ \text{C}$. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, chromium, iron, and silicon; and 0.001 to 0.01 percent each of magnesium, molybdenum, and antimony.

The sample had a light green color. The index of refraction was too high to be measured by the usual oil immersion method.

Interplanar spacings and intensity measurements.

The indices of the three strongest lines are as follows:

Pattern	1	2	3
National Bureau of Standards.....	311	440	220

Structural data. Goldschmidt [1] showed that nickel germanate has the spinel structure, the space group $Fd3m$ (No. 227) and $8(\text{Ni}_2\text{GeO}_4)$ per unit cell.

Goldschmidt's unit cell value has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		<i>A</i>
1931	Goldschmidt.....	8.22
1959	National Bureau of Standards.....	8.221 at 26° C

The density of nickel germanate calculated from the NBS lattice constant is 6.072 g/cm^3 at 26°C .

Nickel Germanate, Ni_2GeO_4 (cubic)

<i>hkl</i>	1959 National Bureau of Standards Cu, 1.5405 Å at 26°C		
	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>
220	2.908	44	8.225
311	2.479	100	8.222
222	2.374	8	8.223
400	2.0558	19	8.223
422	1.6786	17	8.223
511	1.5821	34	8.221
440	1.4533	45	8.221
620	1.3001	6	8.223
533	1.2536	11	8.220
622	1.2392	4	8.220
642	1.0985	7	8.220
731	1.0704	16	8.222
800	1.0277	7	8.222
822	0.9690	4	8.222
751	.9494	10	8.222
840	.9193	2	8.222
664	.8764	3	8.221
931	.8619	6	8.220
844	.8392	16	8.222
10·2·0	.8062	6	8.222
951	.7948	9	8.221
Average value of last five lines		-----	8.221

References

- [1] V. M. Goldschmidt, Zur Kristallchemie des Germaniums, *Nachr. Ges. Wiss. Göttingen, Math.-Physik. Kl.* 184-190 (1931).

Potassium Borohydride, KBH₄ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
8-227	3.33 3.84 2.36	Copper	Banus, Bragdon, and Hinckley [1] 1954.

Additional published patterns. None.

NBS sample. The sample of potassium borohydride was obtained from Metal Hydrides Inc., Beverly, Mass. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent sodium; 0.01 to 0.1 percent strontium; and 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, lead, and silicon.

The sample is colorless. The index of refraction is 1.493.

Interplanar spacings and intensity measurements. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Banus, Bragdon, and Hinckley-----	200	111	220
National Bureau of Standards-----	200	220	111

Structural data. Abrahams and Kalnajs [2] in 1954 determined that potassium borohydride has sodium chloride-type structure, the space group Fm3m (No. 225) and 4(KBH₄) per unit cell.

Lattice constants

Year	Source	A
1954	Abrahams and Kalnajs [2]-----	6.7272 at 25° C
1954	Ford and Powell [3]-----	6.722 at 20° C
1959	National Bureau of Standards-----	6.7287 at 25° C

Potassium Borohydride, KBH₄ (cubic)

hkl	1954 Banus, Bragdon, and Hinckley Cu, 1.542 Å			1959 National Bureau of Standards Cu, 1.5405 Å at 25° C		
	d	I	a	d	I	a
	A		A	A		A
111	3.84	70	6.65	3.883	56	6.726
200	3.33	100	6.66	3.366	100	6.732
220	2.36	70	6.68	2.379	59	6.729
311	2.02	70	6.70	2.029	34	6.729
222	1.925	30	6.68	1.942	19	6.727
400	1.675	10	6.70	1.682	7	6.728
331	1.540	20	6.71	1.543	10	6.726
420	1.500	20	6.71	1.504	19	6.726
422	1.375	20	6.74	1.373	12	6.731
511	1.300	10	6.76	1.295	7	6.732
440	1.195	10	6.76	1.189	4	6.726
531	-----	---	-----	1.137	4	6.727
600	-----	---	-----	1.121	5	6.726
620	-----	---	-----	1.064	5	6.729
533	-----	---	-----	1.0261	2	6.7286
622	-----	---	-----	1.0143	3	6.7288
444	-----	---	-----	0.9712	2	6.7287
711	-----	---	-----	.9422	2	6.7287
640	-----	---	-----	.9331	3	6.7287
642	-----	---	-----	.8991	4	6.7283
731	-----	---	-----	.8760	4	6.7287
800	-----	---	-----	.8411	3	6.7288
733	-----	---	-----	.8220	1	6.7284
820	-----	---	-----	.8160	4	6.7289
822	-----	---	-----	.7930	4	6.7288
Average value of last five lines-----			6.74	-----	---	6.7287

The density of potassium borohydride calculated from the NBS lattice constant is 1.176 g/cm³ at 25° C.

References

- [1] M. B. Banus, R. W. Bragdon, and A. A. Hinckley, Potassium, rubidium, and cesium borohydrides, *J. Am. Chem. Soc.* **76**, 3848-3849 (1954).
- [2] S. C. Abrahams and J. Kalnajs, The lattice constants of the alkali borohydrides and the low-temperature phase of sodium borohydride, *J. Chem. Phys.* **22**, No. 3, 434-436 (1954).
- [3] P. T. Ford and H. M. Powell, The unit cell of potassium borohydride, KBH₄, at 90°K, *Acta Cryst.* **7**, 604-605 (1954).

Potassium Cobaltinitrite, $K_3Co(NO_2)_6$ (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation
Ferrari and Colla [1] 1933.....	Iron

NBS sample. The sample of potassium cobaltinitrite was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent nickel; 0.01 to 0.1 percent each of copper, lead, and rubidium; and 0.001 to 0.01 percent each of aluminum, barium, iron, sodium, silicon, and strontium.

The color of the sample is greenish yellow. The index of refraction is 1.72.

Interplanar spacings and intensity measurements. The d -values reported by Ferrari and Colla have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Ferrari and Colla.....	422	642	400
National Bureau of Standards.....	400	422	220

Structural data. van Driel and Verweel [2] in 1936 determined that potassium cobaltinitrite has the space group Fm3 (No. 202), and $4[K_3Co(NO_2)_6]$ per unit cell. Potassium cobaltinitrite is used as a structure-type.

The unit-cell measurements reported by Ferrari and Colla and by van Driel and Verweel have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1933	Ferrari and Colla [1].....	10.46
1936	van Driel and Verweel [2].....	10.48
1959	National Bureau of Standards.....	10.512 at 25° C

Potassium Cobaltinitrite, $K_3Co(NO_2)_6$ (cubic)

hkl	1933			1958		
	Ferrari and Colla			National Bureau of Standards		
	Fe, 1.937 Å			Cu, 1.5405 Å at 25° C		
	d	I	a	d	I	a
	A		A	A		A
111	-----	---	-----	6.07	31	10.514
200	-----	---	-----	5.257	35	10.514
220	-----	---	-----	3.718	59	10.516
222	-----	---	-----	3.035	26	10.514
400	2.614	s	10.46	2.628	100	10.512
331	-----	---	-----	2.412	12	10.514
420	2.345	s	10.48	2.352	44	10.518
422	2.134	vs	10.46	2.1464	75	10.515
511	2.009	w	10.43	2.0234	14	10.514
440	1.854	w	10.48	1.8585	17	10.513
-----	1.772	vw	-----	-----	---	-----
620	1.658	m	10.48	1.6622	21	10.513
640	1.448	w	10.44	1.4576	11	10.511
642	1.397	vs	10.45	1.4046	32	10.511
800	1.308	w	10.46	1.3145	10	10.516
822	1.238	m	10.50	1.2390	8	10.513
840	1.171	m	10.47	1.1752	14	10.511
644	1.117	m	10.48	1.1204	20	10.510
-----	1.028	s	-----	-----	---	-----
Average value of last five lines.....			10.47	-----	---	10.512

The density of potassium cobaltinitrite calculated from the NBS lattice constant is 2.585 g/cm³ at 25° C.

References

- [1] A. Ferrari and C. Colla, *Ricerche chimiche e cristallografiche sui cobaltinitriti di ammonio, di potassio, di rubidio, di cesio e di talli*, Rend. Accad. Naz. Lincei (6) **17**, 390-398 (1933).
- [2] M. van Driel and H. J. Verweel, *Über die struktur der Tripelnitrite*, Z. Krist. **95A**, 308-314 (1936).

Potassium Heptafluozirconate, K_3ZrF_7 (cubic)

ASTM cards

Additional published patterns

Card number	Index lines	Radiation	Source
3-0511	3.18 2.24 1.83	Molybdenum	Dow Chemical Co., Midland, Michigan.

Source	Radiation
Hampson and Pauling [1] 1938-----	Copper

NBS sample. The sample of potassium heptafluozirconate was contributed by the Titanium Alloy

Potassium Heptafluozirconate, K_3ZrF_7 (cubic)

hkl	Dow Chemical Co. Mo, 0.709 A			1938 Hampson and Pauling Cu, -----			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A
111	5.2	33	9.0	5.17	m-s	8.95	5.190	42	8.989
200	4.50	20	9.0	4.47	m	8.94	4.495	25	8.990
220	3.19	100	9.02	3.16	vvs	8.94	3.177	100	8.986
311	2.72	3	9.02	2.70	vw	8.95	2.710	8	8.988
400	2.24	50	8.96	2.24	s	8.96	2.247	51	8.988
331	2.05	1	8.94	2.05	vw	8.94	2.062	5	8.988
420	2.00	6	8.94	2.00	w	8.94	2.009	12	8.985
422	1.83	50	8.96	1.86	vs	9.11	1.835	48	8.990
511	1.73	10	8.99	1.72	m	8.96	1.729	13	8.984
440	1.59	13	8.99	1.58	m-s	8.96	1.589	15	8.989
531	1.52	3	8.99	1.52	w-m	8.99	1.519	7	8.986
600	1.50	3	9.00	1.50	w	9.00	1.498	5	8.988
620	1.42	13	8.98	1.42	m-s	8.98	1.421	12	8.987
533	1.37	1	8.98	1.37	vvw	8.98	1.371	3	8.990
622	-----	-----	-----	-----	-----	-----	1.355	1	8.988
444	1.29	3	8.94	1.30	vw	8.97	1.2971	6	8.987
711	1.26	1	9.00	1.26	vvw	9.00	1.2584	4	8.987
640	1.25	1	9.01	1.24	<vvw	8.96	1.2466	3	8.989
642	1.19	13	8.90	1.20	m-s	8.99	1.2011	12	8.988
731	1.17	4	8.99	1.17	vw	8.99	1.1702	5	8.988
800	-----	-----	-----	1.12	vvw	8.98	1.1242	3	8.994
733	-----	-----	-----	-----	-----	-----	1.0981	2	8.988
820	-----	-----	-----	1.09	vvw	9.00	1.0900	2	8.988
822	-----	-----	-----	1.06	m	8.99	1.0594	5	8.989
751	-----	-----	-----	1.04	vvw	8.97	1.0379	3	8.989
662	-----	-----	-----	-----	-----	-----	1.0308	3	8.986
840	-----	-----	-----	1.003	w	8.97	1.0048	4	8.987
911	-----	-----	-----	0.985	vw	8.97	0.9867	5	8.989
842	-----	-----	-----	.979	vvw	8.97	.9807	2	8.988
664	-----	-----	-----	.956	vvw	8.97	.9581	1	8.988
931	-----	-----	-----	.942	vvw	8.98	.9422	3	8.988
844	-----	-----	-----	.918	vw	8.99	.9173	3	8.988
933	-----	-----	-----	.905	vw	9.00	.9033	3	8.988
10·2·0	-----	-----	-----	.881	m-s	8.98	.8815	4	8.990
Average value of last five lines---			8.97	-----	-----	8.98	-----	-----	8.988

Mfg. Division of the National Lead Co., Niagara Falls, N. Y. Their spectrographic analysis showed the following impurities: 0.01 to 0.05 percent each of aluminum, iron, hafnium, magnesium, and strontium; 0.004 percent titanium; and 0.0001 to 0.0002 percent each of copper and manganese.

The sample is colorless. The index of refraction was too low to be determined by the grain-immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by the Dow Chemical Co. were converted from kX to angstrom units and the *d*-values reported by Hampson and Pauling were calculated from Bragg angle data. The *i* dice of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Dow Chemical Co.-----	220	400	422
Hampson and Pauling-----	220	422	400
National Bureau of Standards-----	220	400	422

Structural data. Hampson and Pauling [1] in 1938 determined that potassium heptafluozirconate has the space group Fm3m (No. 225), and 4(K₃ZrF₇) per unit cell. The unit-cell measurement reported by Hampson and Pauling has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		<i>A</i>
1938	Hampson and Pauling [1]-----	8.969 (8.98) ^a
1959	National Bureau of Standards-----	8.988 at 25° C

^a Average of last five lines in table.

The density of potassium heptafluozirconate calculated from the NBS lattice constant is 2.209 g/cm³ at 25° C.

References

- [1] G. C. Hampson and L. Pauling, The structure of ammonium heptafluozirconate and potassium heptafluozirconate and the configuration of the heptafluozirconate group, *J. Am. Chem. Soc.* **60**, 2705-2707 (1938)

Praseodymium Oxychloride, PrOCl (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of praseodymium oxychloride was prepared at the NBS by heating praseodymium chloride to 800° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of iron and silicon; and 0.001 to 0.01 percent each of aluminum, calcium, copper, magnesium, and nickel.

The sample has a pale green color. The indices of refraction are *N*_o=1.916 and *N*_e=1.975.

Interplanar spacings and intensity measurements. The indices of the three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards-----	102	101	110

Structural data. Zachariasen [1] in 1949 determined that praseodymium oxychloride has lead fluorochloride-type structure, the space group P4/nmm (No. 129), and 2(PrOCl) per unit cell.

The unit-cell measurements reported by Zachariasen have been converted from kX to angstrom units for comparison with the NBS values.

<i>hkl</i>	1959	
	National Bureau of Standards	
	Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>
	<i>A</i>	
001	6.80	32
101	3.48	90
002	3.397	12
110	2.864	81
102	2.605	100
003	2.266	8
112	2.189	28
200	2.024	41
103	1.977	7
201	1.941	7
113	1.778	22
211	1.751	29
004	1.7001	2
212	1.5985	37
104	1.5676	15
203	1.5100	8
114	1.4623	6
220	1.4322	12
301	1.3245	4
222	1.3204	5
310	1.2811	10
302	1.2547	7
214	1.2395	12
115	1.2290	3
223	1.2100	5

Praseodymium Oxychloride, PrOCl (tetragonal)

<i>hkl</i>	1959	
	National Bureau of Standards	
	Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>
	<i>A</i>	
312	1.1987	8
205	1.1297	5
313	1.1158	8
321	1.1087	5
215	1.0875	3
322	1.0668	9
304	1.0574	6
116	1.0544	3
314	1.0235	4
400	1.0127	2
206	0.9894	5
225	.9865	4
411	.9723	5
330	.9555	4
107	.9443	5
412	.9437	8
324	.9373	5

Lattice constants

		<i>a</i>	<i>c</i>
		<i>A</i>	<i>A</i>
1949	Zachariasen [1]-----	4.053	6.800
1959	National Bureau of Standards-----	4.051	6.802 at 25° C

The density of praseodymium oxychloride calculated from the NBS lattice constants is 5.722 g/cm³ at 25° C.

References

- [1] W. H. Zachariasen, Crystal chemical studies of the 5f-series of elements. XII. New Compounds representing known structure types, *Acta Cryst.* 2, 388-390 (1949).

gamma-Silver Iodide, γ-AgI (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0503	3.74 2.29 1.95	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Barth and Lunde [2] 1925-----	Copper

The color of the sample is bright yellow. The index of refraction is too high to be measured by the usual liquid immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel and reported by Barth and Lunde were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel-----	111	220	311
Barth and Lunde-----	220	311	111
National Bureau of Standards-----	111	220	311

NBS sample. The sample silver iodide was made at the NBS by dissolving Ag₂O in HI. The sample was heated at 120°C for 24 hr to sharpen the diffraction pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon; and 0.001 to 0.01 percent each of aluminum, barium, calcium, copper, iron, magnesium, and sodium.

Structural data. Wilsey [3] in 1921 determined that gamma-silver iodide has the zinc sulfide, zinc-blende, type structure, the space group F43m (No. 216), and 4(AgI) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

gamma-Silver Iodide, γ -AgI (cubic)

<i>hkl</i>	1938			1925			1959		
	Hanawalt, Rinn, and Frevel			Barth and Lunde			National Bureau of Standards		
	Mo, 0.7107 Å			Cu, 1.539 Å			Cu, 1.5405 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
111	3.75	100	6.50	3.76	60	6.51	3.75	100	6.49
220	2.29	75	6.48	2.30	100	6.50	2.30	58	6.50
311	1.95	40	6.47	1.97	90	6.53	1.959	31	6.498
400	1.62	5	6.48	1.63	10	6.52	1.623	4	6.494
331	1.485	8	6.473	1.493	30	6.508	1.490	6	6.494
422	1.321	8	6.472	1.324	40	6.486	1.326	7	6.496
511	1.247	5	6.480	1.254	30	6.516	1.250	5	6.496
440	1.145	3	6.477	1.154	20	6.528	1.148	3	6.494
531	1.096	3	6.484	1.099	50	6.502	1.098	3	6.496
620	-----	-----	-----	1.026	20	6.489	1.027	2	6.495
-----	-----	-----	-----	0.990	20	-----	-----	-----	-----
-----	-----	-----	-----	.943	10	-----	-----	-----	-----
-----	-----	-----	-----	.910	30	-----	-----	-----	-----
642	-----	-----	-----	-----	-----	-----	0.868	2	6.496
Average value of last five lines	-----	-----	6.477	-----	-----	6.504	-----	-----	6.495

Lattice constants

		<i>A</i>
1922	Davey [4]-----	6.53
1925	Barth and Lunde [2]-----	6.504
1925	Wilsey [5]-----	6.506
1931	Block and Möller [6]-----	6.50
1934	Kolkmeijer and van Hengel [7]-----	6.49
1940	Wilman [8]-----	6.502
1948	Mehmel [9]-----	6.48
1950	Trillat and Laloeuf [10]-----	6.49
1959	National Bureau of Standards-----	6.495 at 25° C

The density of gamma-silver iodide calculated from the NBS lattice constant is 5.686 g/cm³ at 25° C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, *Ind. Eng. Chem., Anal. Ed.* **10**, 451-512 (1938).

- [2] T. Barth and G. Lunde, Lattice constants of the cuprous and silver halides, *Norsk. Geol. Tidsskr.* **8**, 281-292 (1925).
- [3] R. B. Wilsey, The crystal structure of the silver halides, *Phil. Mag.* **42**, 262-263 (1921).
- [4] W. P. Davey, The absolute sizes of certain monovalent and bivalent ions, *Phys. Rev.* **19**, 248-251 (1922).
- [5] R. B. Wilsey, X-ray analysis of some mixed crystals of the silver halides, *J. Franklin Inst.* **200**, 739-746 (1925).
- [6] R. Block and H. Möller, Über die Modifikationen des Jodsilbers, *Z. physik. Chem.* **152A**, 245-268 (1931).
- [7] N. H. Kolkmeijer and J. W. A. van Hengel, Über das reguläre und das hexagonale Silberjodid, *Z. Krist.* **88**, 317-322 (1934).
- [8] H. Wilman, The structure and orientation of silver halides, *Proc. Phys. Soc. (London)* **52**, 323-347 (1940).
- [9] M. Mehmel, Kristallchemische Betrachtungen zur I. und VII. Gruppe des periodischen Systems der Elemente, *Optik* **3**, 41-46 (1948).
- [10] J. J. Trillat and A. Laloeuf, Etude par diffraction électronique, de la structure des fumées d'iodure d'argent et de chlorure d'ammonium, *Rayons X et structure atomique*, 19-29 (1950).

Silver Metaperiodate, AgIO₄ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
4-0559	3.21 1.64 1.30	Iron	Birkenbach and Buschendorf [1] 1932.

Additional published patterns. None.

NBS sample. The sample of silver metaperiodate was prepared at the NBS from cold solutions of silver nitrate and sodium metaperiodate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum and silicon; and 0.001 to 0.01 percent each of beryllium, calcium, cobalt, chromium, iron, indium, magnesium, molybdenum, and nickel.

The color of the sample was tan. The indices of

refraction could not be determined because the sample was too fine-grained.

Interplanar spacings and intensity measurements.

The d -values reported by Birkenbach and Buschendorf were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Birkenbach and Buschendorf..	303, 312	503, 512	103, 112
National Bureau of Standards..	103, 112	204	004

Structural data. Birkenbach and Buschendorf [1] in 1932 determined that silver metaperiodate has scheelite-type structure, the space group $I4_1/a$ (No. 88) and $4(\text{AgIO}_4)$ per unit cell.

The unit-cell measurements reported by Birkenbach and Buschendorf have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
1932	Birkenbach and Buschendorf.....	A	A
1959	National Bureau of Standards.....	5.379	12.037
		5.374	12.094 at 25° C

The density of silver metaperiodate calculated from the NBS lattice constants is 5.68 g/cm^3 at 25°C .

References

- [1] L. Birkenbach and F. Buschendorf, Darstellung und Kristallstruktur des normalen (meta-) Silberperiodats, *Z. physik. Chem.* **B16**, 102-112 (1932).

Silver Metaperiodate, AgIO_4 (tetragonal)

hkl	1932		1959	
	Birkenbach and Buschendorf		National Bureau of Standards	
	Fe, 1.937 A		Cu, 1.5305 A at 25°C	
	d	I	d	I
	A		A	
101	-----	-----	4.91	9
103	3.22	vs	3.22	100
112				
004	3.02	vw	3.02	22
200	2.69	w	2.687	21

hkl	1932		1959	
	Birkenbach and Buschendorf		National Bureau of Standards	
	Fe, 1.937 A		Cu, 1.5305 A at 25°C	
	d	I	d	I
	A		A	
114	2.36	vww	2.366	5
211			2.358	5
204			2.007	30
220			1.899	14
116	1.778	vs	1.781	16
301				
215	-----	-----	1.703	3
303	1.637	vvs	1.635	20
312				
224				
008				
314	1.478	vww	1.475	1
321				
118				
400				
208	1.317	w	1.318	6
316	1.299	vs	1.299	8
413	1.240	m	1.240	6
332				
404				
420				
228	1.181	s	1.183	5
1-1-10	1.148	vw	1.153	6
406	1.118	vs	1.119	7
424			1.117	7
309			1.074	4
336			1.0728	3
503	1.036	vvs	1.0384	6
512				
0-0-12				
408				
3-1-10	-----	-----	0.9856	3
440	-----	-----	.9505	3
2-0-12	-----	-----	.9438	5
428	-----	-----	.9408	5
419	-----	-----	.9341	6
516				
532	-----	-----	.9112	8
444	-----	-----	.9064	7
600	-----	-----	.8954	4
2-2-16	-----	-----	.8905	5
3-3-10	-----	-----	.8749	3
446	-----	-----	.8587	2
604				
620				
622				
1-1-14	-----	-----	.8407	1
536	-----	-----	.8381	3
541				
606				
624				
4-0-12	-----	-----	.8062	3
448	-----	-----	.8043	3
5-1-10	-----	-----	.7945	4

Sodium Borohydride, NaBH₄ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of sodium borohydride was obtained from T. B. Douglas at NBS. Chemical analysis indicated the following percentages of the theoretical: sodium, 99.9 percent; boron, 99.9 percent; and hydrogen, 99.4 percent.

The sample is white. The indices of refraction could not be determined because the sample reacted violently with the index liquids.

Interplanar spacings and intensity measurements. The indices of the three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards.....	200	220	111

Structural data. Soldate [1] in 1947 determined that the location of the Na and B atoms is of the NaCl type, but the positions of the hydrogen atoms and hence the space group could not be settled. The lattice is face-centered cubic with 4(NaBH₄) assumed per unit cell.

Lattice constants

1959	National Bureau of Standards.....	$\frac{A}{6.162 \text{ at } 25^\circ \text{ C}}$
------	-----------------------------------	--

The density of sodium borohydride calculated from the NBS lattice constant is 1.074 g/cm³ at 25° C.

Strontium Zirconate, SrZrO₃ (orthorhombic)

ASTM cards

Card numbers ^a	Index lines	Radiation	Source
1-0937	2.90 1.67 2.04	Molybdenum	New Jersey Zinc Co.
2-1447	1.09 2.89 2.04	Copper	Hoffmann [1] 1935.
3-0684	2.90 1.68 1.10	—	Megaw.

^a These cards are listed as cubic.

<i>hkl</i>	1959 National Bureau of Standards Cu, 1.5405 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>
	$\frac{A}{\text{Å}}$		$\frac{A}{\text{Å}}$
111	3.55	25	6.16
200	3.082	100	6.163
220	2.181	48	6.168
311	1.857	19	6.160
222	1.778	13	6.160
400	1.540	4	6.161
331	1.414	3	6.164
420	1.3781	10	6.163
422	1.2577	7	6.161
511	1.1855	3	6.160
440	1.0895	2	6.163
531	1.0416	1	6.162
600	1.0270	3	6.162
620	0.9742	2	6.161
533	.9398	<1	6.163
622	.9289	2	6.162
444	.8893	<1	6.161
711	.8630	<1	6.163
640	.8543	2	6.161
642	.8234	3	6.161
Average value of last five lines		-----	6.162

References

- [1] A. M. Soldate, The crystal structure of sodium borohydride, *J. Am. Chem. Soc.* **69**, 987-988 (1947).

Additional published patterns

Source	Radiation
Zachariasen [2] 1928.....	Iron

NBS sample. The sample of strontium zirconate was prepared at NBS by R. S. Roth. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of hafnium, aluminum, silicon, calcium and barium; 0.01 to 0.1 percent each of iron, magnesium, and titanium; and 0.001 to 0.01 percent each of beryllium and nickel.

The color of the sample was pinkish-white. The indices of refraction were too high to be determined

by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The d -values reported by the New Jersey Zinc Co., by Megaw, and by Zachariasen were converted from kX to angstrom units and the pattern reported by Hoffman was calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
New Jersey Zinc Co.-----	121, 002	{321, 123, 042	202, 040
Hoffmann-----	{521, 244, 125, 163	121, 002	202, 040
Megaw-----	121, 002	{321, 123, 042	{521, 244, 125, 163
Zachariasen-----	{521, 244, 125, 163	{321, 123, 042	121, 002
National Bureau of Standards--	002	121	202, 040

Structural data. The structure of strontium zirconate has not been published. Megaw [3] in 1946 showed some of the perovskite-type compounds to be orthorhombic. Roth [4] in 1957 reported that the probable symmetry of strontium zirconate was orthorhombic. Bailey [5], as quoted by Megaw [6], used the $CaTiO_3$ space group, $Pnma$ (No. 62), and $4(SrZrO_3)$ per unit cell.

Lattice constants

		a	b	c
		$\text{\AA}$	$\text{\AA}$	$\text{\AA}$
1957	Roth [4]-----	5.818	8.189	5.792
1959	National Bureau of Standards-----	5.814	8.196	5.792 at 25° C

The density of strontium zirconate calculated from the NBS lattice constants is 5.458 g/cm^3 at 25°C .

Strontium Zirconate, $SrZrO_3$ (orthorhombic)

hkl	----- New Jersey Zinc Co. Mo, -----		1935 Hoffmann Cu, -----		----- Megaw -----		1928 Zachariasen Fe, -----		1959 National Bureau of Standards Cu, 1.5405 $\text{\AA}$ at 25°C	
	d	I	d	I	d	I	d	I	d	I
	$\text{\AA}$		$\text{\AA}$		$\text{\AA}$		$\text{\AA}$		$\text{\AA}$	
020	-----	-----	-----	-----	-----	-----	-----	-----	4.096	5
111	-----	-----	-----	-----	-----	-----	-----	-----	3.666	5
121	} 2.91	100	2.90	90	2.91	100	2.90	50	{ 2.900	67
002										
210										
	-----	-----	-----	-----	-----	-----	-----	-----	2.895	100
	-----	-----	-----	-----	-----	-----	-----	-----	2.735	1
201	-----	-----	-----	-----	-----	-----	-----	-----	2.598	2
102	-----	-----	-----	-----	-----	-----	-----	-----	2.590	2
112	}	-----	-----	-----	-----	-----	-----	-----	2.469	4
031										
220										
	-----	-----	-----	-----	-----	-----	-----	-----	2.369	4
022	-----	-----	-----	-----	-----	-----	-----	-----	2.363	1
131	-----	-----	-----	-----	-----	-----	-----	-----	2.272	<1
221	}	-----	-----	-----	-----	-----	-----	-----	2.191	<1
122										
202										
040										
	2.04	40	2.04	80	2.05	70	2.04	40	2.050	41
212	}	-----	-----	-----	-----	-----	-----	-----	1.986	3
230										
231										
132, 013										
	-----	-----	-----	-----	-----	-----	-----	-----	1.880	3
301	}	-----	-----	-----	-----	-----	-----	-----	1.837	3
222										
103										
141										
311	-----	-----	-----	-----	-----	-----	-----	-----	1.792	2
321	}	-----	-----	-----	-----	-----	-----	-----	1.676	22
123										
042										
232										
213	1.67	67	1.67	80	1.68	80	1.67	70	1.672	36
	-----	-----	-----	-----	-----	-----	-----	-----	1.6388	<1
	-----	-----	-----	-----	-----	-----	-----	-----	1.5785	<1

<i>hkl</i>	----- New Jersey Zinc Co. Mo, -----		1935 Hoffmann Cu, -----		----- Megaw -----		1928 Zachariasen Fe, -----		1959 National Bureau of Standards Cu, 1.5405 Å at 25°C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	<i>A</i>		<i>A</i>		<i>A</i>		<i>A</i>		<i>A</i>	
331									1.5246	1
400	} 1.45	27	1.45	60	1.45	70	1.45	40	1.4527	6
242									1.4495	14
410									1.4306	1
233									1.3860	1
303	}	24	1.29	70	1.30	70	1.30	50	1.3679	1
341									1.3489	<1
313									1.2966	12
204									1.2830	1
412	}								1.2799	1
430									1.2230	1
214									1.1854	5
252									1.1826	5
333	}	3	1.18	40	1.18	50	1.18	20	1.1731	1
351									1.1289	1
440									1.0980	8
044									1.0951	13
432	}	27	1.09	100	1.10	80	1.09	100	1.0522	2
511									1.0254	4
521									1.0177	<1
244									0.9962	<1
125, 163	}		1.02	60					.9940	<1
531									.9884	<1
404									.9675	4
414									.9665	8
452	}				0.967	70			.9359	2
503									.917	70
541									.9187	3
305									.9169	5
145	}								.9134	2
513									.8756	3
523									.8735	4
325									.8514	1
363	}								.8385	5
533									.8364	3
551									.8181	2
602									.8062	4
444	}				.837	70			.8042	10
612										
630										
640										
165	}				.875	70				
046										
553										
642										
246	}				.804	80				
084										
711										
721										
406	}									
482										

References

- [1] A. Hoffmann, Untersuchungen über Verbindungen mit Perowskitstruktur, *Z. physik Chem.* **28B**, 65-67 (1935).
- [2] W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxiden und Verbindungen ABO_3 , *Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. 4* (1928).
- [3] H. D. Megaw, Crystal structure of double oxides of the

perovskite type, *Proc. Phys. Soc. London* **58**, 133-152 (1946).

- [4] R. S. Roth, Classification of perovskite and other ABO_3 -type compounds, *J. Research Nat. Bur. Standards* **58**, No. 2, 75-88 (1958).
- [5] P. Bailey, Thesis, Bristol (1952).
- [6] H. D. Megaw, Ferroelectricity and crystal structure. II, *Acta Cryst.* **7**, 187-194 (1954).

Sulfur, S (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
8-247, 8-248	3.85 3.21 3.44	Copper	deWolff, Delft, Holland

Structural data. Mark and Wigner [3] in 1924 determined that alpha sulfur has the space group $Fddd$ (No. 70) and 128(S) per unit cell. Sulfur is used as a structure-type.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		<i>A</i>	<i>A</i>	<i>A</i>
1924	Mark and Wigner [3]-----	10.63	12.89	24.61
1925	Bragg and Bragg [4]-----	10.48	12.89	24.51
1935	Warren and Burwell [5]-----	10.50	12.95	24.60
1937	Trillat and Oketani [6]-----	10.42	12.83	24.60
1951	Ventriglia [7]-----	10.48	12.92	24.55
1955	Abrahams [8]-----	10.437	12.845	24.369
1958	deWolff-----	10.45	12.84	24.46
1959	National Bureau of Standards-----	10.468	12.870	24.49 at 25° C

The density of sulfur calculated from the NBS lattice constants is 2.065 g/cm³ at 25° C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, *Ind. Eng. Chem., Anal. Ed.* **10**, 457-512 (1938).
- [2] S. R. Das, A study of sulfur allotropes by X-ray diffraction method, *Indian J. Phys.* **12**, 163-181 (1938).
- [3] H. Mark and E. Wigner, Die Gitterstruktur des rhombischen Schwefel, *Z. physik. Chem.* **111**, 398-414 (1924).
- [4] W. H. Bragg and W. L. Bragg, X-rays and Crystal Structure, Fifth Ed., London, Bell, 254-257 (1925).
- [5] B. E. Warren and J. T. Burwell, The structure of rhombic sulfur, *J. Chem. Phys.* **3**, 6-8 (1935).
- [6] J. J. Trillat and S. Oketani, Étude sur la structure du soufre au moyen des rayons cathodiques, *Z. Krist. (A)* **98**, 334-343 (1937).
- [7] U. Ventriglia, Sulla struttura dello zolfo rombico, *Periodico mineral. (Rome)* **20**, 237-55 (1951).
- [8] S. G. Abrahams, The crystal and molecular structure of orthorhombic sulphur, *Acta Cryst.* **8**, 661-671 (1955).

Additional published patterns

Source	Radiation
Hanawalt, Rinn, and Frevel ^a [1]----- Das [2]-----	Molybdenum -----

^a ASTM card deleted in 8th Ed. Card Index.

NBS sample. The sample of sulfur was purified by Meyer Waxman at NBS. The sample was ground and annealed at 85° C to sharpen the diffraction pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent sodium; 0.001 to 0.01 percent each of barium, magnesium, and silicon; and 0.0001 to 0.001 percent calcium.

The color of the sample was yellow and it was optically positive. The index of refraction, $N_\alpha = 1.957$; N_β and N_γ were too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel and by Das have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel-----	222	206, 040	313
Das-----	222	026	206, 040, 313
deWolff-----	222	206, 040	026
National Bureau of Standards-----	222	206, 040	026

Sulfur, S (orthorhombic)

<i>hkl</i>	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 Å		1938 Das -----		1958 deWolff Cu, 1.5405 Å		1959 National Bureau of Standards Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>d</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	<i>A</i>		<i>A</i>		<i>A</i>		<i>A</i>	
111	-----	-----	-----	-----	7.69	6	7.72	9
113	-----	-----	-----	-----	5.76	14	5.78	17
022	5.8	31	5.67	ms	5.68	5	5.70	8
202	-----	-----	-----	-----	4.80	2	4.82	4
115	-----	-----	-----	-----	4.19	2	4.20	5
220	-----	-----	-----	-----	4.06	11	4.062	15
131	-----	-----	-----	-----	3.91	12	3.921	20
222	3.86	100	3.85	vs	3.85	100	3.859	100
133	-----	-----	-----	-----	3.57	8	3.571	11
026	3.46	31	3.46	s	3.44	40	3.450	42
224	-----	-----	-----	-----	3.38	3	3.387	4
311	-----	-----	-----	-----	3.33	25	3.336	23
206	3.22	50	3.15	s	3.21	60	3.220	50
040					3.11	25	3.115	26
313	3.11	38						
135	-----	-----	-----	-----	3.08	17	3.087	15
008	-----	-----	-----	-----	3.06	1	-----	-----
044	-----	-----	2.85	ms	2.842	18	2.848	23
331	-----	-----	-----	-----	2.688	2	2.690	3
242	-----	-----	-----	-----	2.673	1	2.673	1
137	2.64	20	2.65	w	2.621	13	2.624	14
400	-----	-----	-----	-----	2.614	4	2.618	9
333	-----	-----	-----	-----	2.569	8	2.570	4
244	2.51	18	-----	-----	2.501	7	2.502	10
151	-----	-----	-----	-----	-----	-----	2.487	4
317	2.43	20	2.41	vw	2.424	13	2.428	15
404	-----	-----	-----	-----	2.404	2	2.407	4
422	2.38	15	2.26	w	2.375	4	2.379	7
335					2.366	4	2.371	6
0·2·10	2.30	15			2.288	6	2.289	5
048	-----	-----	-----	-----	2.215	2	-----	-----
1·1·11	-----	-----	-----	-----	2.146	4	2.146	4
319	2.12	25	2.12	vw	2.112	10B	2.115	11
062					2.098	2	2.113	11
2·2·10	-----	-----	-----	-----	-----	-----	2.096	3
511	-----	-----	-----	-----	2.057	1	2.058	1
248	2.00	3	1.98	vw	2.041	1	2.042	<1
0·0·12					-----	-----	2.008	3
353	2.00	3	1.91	vvw	2.003	2	2.003	3
513					-----	-----	-----	-----
442	-----	-----	-----	-----	1.988	4	1.989	4
408	-----	-----	-----	-----	1.957	2	1.960	4
262	-----	-----	-----	-----	1.926	1	1.926	2
444	1.90	25	1.91	vvw	1.900	7B	1.908	6
355					-----	-----	1.904	9
515	-----	-----	-----	-----	1.856	1	1.857	<1
3·1·11	-----	-----	-----	-----	1.838	1	1.842	<1
159	-----	-----	-----	-----	1.823	4	1.823	2
2·2·12	1.83	18	-----	-----	1.781	11	1.782	10
357	1.78	20	1.79	vvw	1.754	7	1.756	6
535	-----	-----	-----	-----	-----	-----	-----	-----

<i>hkl</i>	1938 Hanawalt, Rinn, and Prevel Mo, 0.7107 Å		1938 Das ----		1958 deWolff Cu, 1.5405 Å		1959 National Bureau of Standards Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	<i>A</i>		<i>A</i>		<i>A</i>		<i>A</i>	
602	1.73	18	1.74	vvw	1.725	8	1.727	10
4·2·10	-----	-----	-----	-----	-----	-----	1.723	7
175	-----	-----	-----	-----	1.698	7	1.698	7
268	1.66	10	-----	-----	1.665	2	1.665	3
357	-----	-----	-----	-----	1.658	2	1.657	2
359	-----	-----	-----	-----	1.647	5	1.648	5
462	-----	-----	-----	-----	-----	-----	1.644	3
624	}	-----	-----	-----	1.622	6	1.623	7
371								
551								
-----	-----	-----	-----	-----	-----	-----	1.620	3
080	-----	-----	-----	-----	-----	-----	1.609	1
177	}	20	-----	-----	1.607	6	1.607	2
2·2·14								
1·1·15								
464	-----	-----	-----	-----	1.601	2	1.601	1
373	}	-----	-----	-----	1.595	3	1.595	2
553								
4·4·10								
4·2·12	-----	-----	-----	-----	1.563	2	1.563	1
2·6·10	}	3	-----	-----	1.542	1	1.542	<1
555								
466					1.531	1	1.537	<1
5·1·11	-----	-----	-----	-----	1.515	1	-----	-----
1·5·13	-----	-----	-----	-----	1.504	1	1.504	1
284	-----	-----	-----	-----	1.490	1	1.4914	1
644	-----	-----	-----	-----	-----	-----	1.4875	1
628	}	3	-----	-----	1.475	2	1.4756	2
2·4·14								
377								
713	-----	-----	-----	-----	1.461	1	1.4617	1
286	1.44	10	-----	-----	1.439	3	1.4389	1
646	1.43	15	-----	-----	-----	-----	1.4359	1
2·6·12	-----	-----	-----	-----	1.424	3	1.4230	2
1·1·17	}	-----	-----	-----	1.419	1	1.4194	3
4·2·14								
733	-----	-----	-----	-----	1.391	1	1.3911	1
6·2·10	-----	-----	-----	-----	-----	-----	1.3879	<1
480	-----	-----	-----	-----	-----	-----	1.3702	<1
573	}	13	-----	-----	1.362	1	1.3620	<1
482								
0·6·14	-----	-----	-----	-----	-----	-----	1.3561	1
660	(*)	-----	-----	-----	1.354	3	1.3536	2

* Two additional lines were omitted.

Tellurium(IV) Oxide, (tellurite), TeO₂ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0117	6.8 2.82 3.09	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of tellurite, U. S. National Museum #R 8861, was obtained originally from Cananea, Sonora, Mexico. Attempts to synthesize the orthorhombic form were unsuccessful. Spectrographic analysis obtained from the U. S. Geological Survey showed the following impurities: 0.5 percent silicon; 0.3 percent copper; 0.2 percent each of aluminum and barium; 0.1 percent each of calcium and magnesium; 0.08 percent iron; 0.05 percent each of bismuth and tin; 0.02 percent each of lead, manganese, and strontium; and 0.004 percent silver.

The sample is colorless and optically positive. The refractive indices are too high to be measured by the usual liquid immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The mineral has a platy cleavage which has been identified with the 010 plane. If intensity measurements are obtained from a pressed sample the 040 reflection will dominate the pattern, being considerably stronger than any other line. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	020	131, 200	040
National Bureau of Standards	121	111	040

Structural data. Ito and Sawada [2] in 1939 determined that tellurite has the space group Pbca (No. 61) and 8(TeO₂) per unit cell. Tellurite is used as a structure-type.

The unit-cell measurements reported by Ito and Sawada have been converted from kX to angstrom units for comparison with the NBS values.

<i>hkl</i>	1938		1959	
	Hanawalt, Rinn, and Frevel		National Bureau of Standards	
	Mo, 0.7107 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	<i>A</i>		<i>A</i>	
020	6.81	100	6.01	5
021	4.27	13	4.05	10
111	3.89	10	3.723	94
	3.42	44		
121	3.24	50	3.280	100
040	3.10	63	3.008	47
131	2.83	75	2.800	24
200				
002			2.730	44
210				
041			2.636	4
102			2.453	9
221	2.29	31	2.298	24
230	2.17	3		
	2.12	5		
240	2.07	3	2.050	21
151			2.023	20
042	1.93	8	1.930	26
212				
061			1.883	2
250	1.83	20	1.826	8
161	1.78	15	1.785	17
232			1.759	21
311	1.73	20	1.750	16
113			1.714	9
321			1.696	17
123			1.666	8
062	164	8	1.6168	6
331	1.58	10	1.5903	7
133				
171	1.55	3	1.5734	2
252	1.51	13	1.5176	10
213				
080			1.5021	2
143				
270	1.440	4	1.4662	9
351			1.4246	5
173	1.407	13	1.4093	6
181			1.4026	7
361	1.359	3	1.3267	8
082	1.315	3	1.3184	6
313			1.2946	11
124				
253	1.281	3	1.2885	5
281				
440			1.2708	7
191			1.2650	3
402			1.2489	6
044			1.2434	5
1·10·1			1.1504	7

		<i>a</i>	<i>b</i>	<i>c</i>
		<i>A</i>	<i>A</i>	<i>A</i>
1939	Ito and Sawada	5.60	11.77	5.51
1959	National Bureau of Standards	5.607	12.034	5.463 at 25° C

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10**, 457-512 (1938).
 [2] T. Ito and H. Sawada, The crystal structure of tellurite (TeO₂), Z. Krist. **102A**, 13-25 (1939).

Thulium(III) Oxide, Tm₂O₃ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2-0631	3.02 1.85 1.58	Copper	Bommer [1] 1939.

Additional published patterns. None.

NBS sample. The sample of thulium sesquioxide was prepared by the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed the following impurities: a total of less than 0.1 percent of erbium and ytterbium oxides and a trace of lutecium oxide. The sample was annealed at 1,100° C for a period of 16 hr.

The sample was colorless. The index of refraction was not determined because the sample was too fine-grained.

Interplanar spacings and intensity measurements. Bragg angle data reported by Bommer was converted to *d*-values in angstroms. The indices of the three strongest lines of each pattern are as follows:

<i>hkl</i>	1939 Bommer			1959 National Bureau of Standards		
	Cu, 1.5418 Å			Co, 1.7889 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
211	-----	---	-----	4.28	16	10.491
222	3.02	vs	10.47	3.028	100	10.490
321	2.809	vw	10.51	2.803	4	10.487
400	2.617	s	10.47	2.622	41	10.489
411	2.468	w	10.47	2.472	8	10.487
420	2.342	vw	10.47	2.3452	3	10.488
332	-----	---	-----	2.2368	5	10.492
422	2.138	vw	10.48	2.1401	2	10.484
431	2.055	m	10.48	2.0570	10	10.489
521	1.912	vw	10.47	1.9147	4	10.487
440	1.850	vs	10.46	1.8534	40	10.484
433	1.795	vw	10.47	1.7989	4	10.489
600	1.744	vw	10.46	1.7478	1	10.487
611	1.698	m	10.47	1.7019	6	10.491
620	1.656	vw	10.47	1.6588	1	10.491

<i>hkl</i>	1939 Bommer			1959 National Bureau of Standards		
	Cu, 1.5418 Å			Co, 1.7889 Å at 25° C		
	<i>d</i>	<i>I</i>	<i>a</i>	<i>d</i>	<i>I</i>	<i>a</i>
	<i>A</i>		<i>A</i>	<i>A</i>		<i>A</i>
541	1.616	w-m	10.47	1.6184	4	10.488
622	1.578	vs	10.46	1.5810	29	10.487
631	1.544	m	10.47	1.5467	6	10.490
444	1.512	m-s	10.48	1.5141	7	10.490
543	1.482	w	10.48	1.4835	3	10.490
640	1.455	vw	10.49	1.4550	1	10.492
721	1.425	w	10.47	1.4281	3	10.494
642	-----	---	-----	1.4016	2	10.489
732	1.331	w	10.48	1.3322	2	10.490
800	1.309	w-m	10.47	1.3114	4	10.491
811	-----	---	-----	1.2917	4	10.494
820	1.270	vw	10.47	1.2722	2	10.491
653	1.252	w	10.47	1.2538	2	10.490
822	1.235	vw	10.48	1.2362	2	10.490
831	1.216	w-m	10.46	1.2195	4	10.490
662	1.202	m-s	10.48	1.2034	8	10.491
840	1.170	m-s	10.47	1.1727	7	10.489
833	1.157	w	10.47	1.1582	1	10.488
842	1.143	w	10.48	1.1445	1	10.490
921	1.129	m	10.47	1.1312	2	10.490
851	1.103	w-m	10.47	1.1058	3	10.490
932	1.0803	w-m	10.474	1.0820	2	10.490
844	1.0693	m-s	10.477	1.0706	6	10.490
941	-----	---	-----	1.0596	3	10.490
10·0·0	-----	---	-----	1.0489	2	10.489
10·1·1	-----	---	-----	1.0386	1	10.489
10·2·0	1.0277	m	10.481	1.0286	4	10.490
943	-----	---	-----	1.0189	1	10.490
10·2·2	1.0082	m-s	10.478	1.0094	5	10.490
10·3·1	-----	---	-----	1.0002	3	10.490
871	-----	---	-----	0.9824	3	10.489
10·4·0	-----	---	-----	.9739	4	10.489
10·3·3	-----	---	-----	.9655	2	10.488
10·4·2	-----	---	-----	.9574	4	10.488
954	-----	---	-----	.94957	3	10.4883
11·2·1	-----	---	-----	.93432	4	10.4877
880	-----	---	-----	.92700	2	10.4878
10·4·4	-----	---	-----	.91289	2	10.4883
11·3·2	-----	---	-----	.90602	2	10.4879
Average value of last five lines			10.476	-----	---	10.4880

Pattern	1	2	3
Bommer-----	222	440	622
National Bureau of Standards-----	222	400	440

Structural data. Pauling and Shappell [4] in 1930 determined that thulium sesquioxide has the thalliumoxide type structure (rare earth type C), the space group Ia3 (No. 206) and 16 (Tm₂O₃) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1925	Goldschmidt, Barth, and Lunde [3]---	10.54
1927	Zachariasen [2]-----	10.54
1939	Bommer [1]-----	10.48
1954	Templeton and Dauben [5]-----	10.488
1959	National Bureau of Standards-----	10.488 at 25° C

Titanium(III) Oxide, TiO_{1.515} (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-1359	1.68 1.85 1.47	Copper	Halla [1] 1929.

Additional published patterns

Source	Radiation
Zachariasen [2] 1928-----	Copper

NBS sample. The sample of titanium sesquioxide was obtained from Linde Speedway Laboratory, Indianapolis, Ind. Spectrographic analysis showed the following impurities. 0.01 to 0.1 percent each of aluminum, cobalt, chromium, iron, and silicon; and 0.001 to 0.01 percent each of barium and copper. Andersson, Collén, Kuylenstierna, and Magnéli [3] reported a homogeneity range in Ti₂O₃ of TiO_{1.49} to TiO_{1.51}. Our chemical analysis showed this sample to have TiO_{1.515}.

The sample is a black opaque powder.

Interplanar spacings and intensity measurements. The *d*-values reported by Halla and by Zachariasen

The density of thulium sesquioxide calculated from the NBS lattice constant is 8.884 g/cm³ at 25° C.

References

- [1] H. Bommer, Die Gitterkonstanten der C-Formen der Oxyde der seltenen Erdmatalle, Z. anorg. u. allgem. Chem. **241**, 273-280 (1939).
- [2] W. Zachariasen, The crystal structure of the modification C of the sesquioxides of the rare earth metals, and of indium and thallium, Norsk Geol. Tidsskr. **9**, 310-316 (1927).
- [3] V. M. Goldschmidt, T. Barth, and G. Lunde, Isomorphie und Polymorphie der Sesquioxide, die Lanthaniden-Kontraktion und ihre Konsequenzen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. 7, 1-59 (1925).
- [4] L. Pauling and M. D. Shappell, The crystal structure of Bixbyite and the C-modification of the sesquioxides, Z. Krist. **75**, 128-142 (1930).
- [5] D. H. Templeton and C. H. Dauben, Lattice parameters of some rare earth compounds and a set of crystal radii, J. Am. Chem. Soc. **76**, 5237-5239 (1954).

<i>hkl</i>	1929 Halla		1928 Zachariasen		1959 National Bureau of Standards	
	Cu, 1.5418 Å		Cu, 1.5418 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	<i>A</i>		<i>A</i>		<i>A</i>	
012	-----	---	3.71	40	3.732	26
104	2.73	w	2.69	50	2.712	52
110	2.57	w	2.57	50	2.572	58
006	-----	---	-----	---	2.277	7
113	2.23	vw	2.24	40	2.238	36
202	-----	---	2.118	10	2.116	10
024	1.869	m	1.858	50	1.865	35
116	1.696	w	1.696	100	1.704	100
	1.688	s	1.668	10	-----	---
122	1.632	vw	1.641	20	1.634	11
018	-----	---	-----	---	1.592	3
214	1.494	w	1.508	40	1.510	31
300	1.481	m	1.484	60	1.483	45
119	1.305	w	1.299	30	1.306	24
220	-----	---	1.287	30	1.2849	16
306	1.241	vw	1.241	30	1.2432	10
223	-----	---	-----	---	1.2365	6
312	-----	---	1.219	10	1.2146	6
0-2-10	1.166	m	-----	---	1.1643	6
134	-----	---	1.161	30	1.1613	16
0-0-12	-----	---	-----	---	1.1386	7
226	1.123	m	1.118	40	1.1192	26
042	-----	---	-----	---	1.0982	4
2-1-10	1.067	m	-----	---	1.0603	10
404	-----	---	1.058	40	1.0578	16

Structural data. Lunde [4] in 1927 determined that titanium sesquioxide has alpha aluminum oxide-type structure, the space group $R\bar{3}c$ (No. 167), and $2(\text{Ti}_2\text{O}_3)$ per unit rhombohedral cell or $6(\text{Ti}_2\text{O}_3)$ per unit hexagonal cell.

Two unit-cell measurements reported in the literature have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>a</i>	<i>c</i>
		<i>A</i>	<i>A</i>
1927	Lunde [4]-----	5.144	13.642
1928	Zachariasen [2]-----	5.16	13.59
1957	Andersson, Collén, Kuylenstierna, and Magnéli [3]---	^a 5.160	13.60
1957	Andersson, Collén, Kuylenstierna, and Magnéli [3]---	^b 5.147	13.64
1959	National Bureau of Standards-----	^c 5.139	13.659 at 25° C

^a $\text{TiO}_{1.49}$
^b $\text{TiO}_{1.51}$
^c $\text{TiO}_{1.515}$

The density of titanium sesquioxide calculated from the NBS lattice constants is 4.585 g/cm^3 at 25° C.

References

- [1] F. Halla, Reaktionen des Titansesquioxids mit Eisenoxyd, *Z. anorg. Chem.* **184**, 421-427 (1929).
- [2] W. H. Zachariasen, The crystal structure of the sesquioxides and compounds of the type ABO_3 , *Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl.* **1928**, No. 4 (1928).
- [3] S. Andersson, B. Collén, U. Kuylenstierna, and A. Magnéli, Phase analysis on the titanium-oxygen system, *Acta Chem. Scand.* **11**, 1641-1652 (1957).
- [4] G. Lunde, Über Titansesquioxid, *Z. anorg. u. allgem. Chem.* **164**, 341-344 (1927).

Zinc Iodide, ZnI_2 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0575	3.49 6.5 2.11	Molybdenum	Hanawalt, Rinn, and Frevel [1], 1938.

Additional published patterns. None.

NBS sample. The sample of zinc iodide was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent phosphorous; 0.01 to 0.1 percent calcium; and 0.001 to 0.01 percent each of aluminum, barium, iron, magnesium, and silicon.

The sample was colorless. The indices of refraction were not measured because the sample reacted with the index liquids.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Halla-----	---	3·0·12	024
Zachariasen-----	116	300	104
National Bureau of Standards--	116	110	104

Zinc Iodide, ZnI₂ (tetragonal)

<i>hkl</i>	1938		1959	
	Hanawalt, Rinn, and Frevel		National Bureau of Standards	
	Mo, 0.7107 Å		Cu, 1.5405 Å at 25° C	
	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>
	<i>A</i>		<i>A</i>	
-----	6.5	20B	-----	-----
-----	5.7	20B	-----	-----
-----	4.5	12	-----	-----
-----	3.99	12	-----	-----
102	3.50	100	3.49	100
110	3.07	8	3.068	21
004	2.94	3	2.945	4
112	2.76	3	2.756	5
104	-----	-----	2.441	3
200	2.17	16	2.169	21
114	2.11	28	2.125	39
105	-----	-----	2.053	4
212	1.84	20	1.843	33
106	1.79	8	1.789	10
204	1.74	4	1.746	12
220	1.53	4	1.534	9
008	-----	-----	1.473	4
302	-----	-----	1.405	8
216	1.378	4	1.380	13
310	-----	-----	1.373	6
224	-----	-----	1.360	3
118	-----	-----	1.3282	3
314	1.242	4	1.2442	10
208	-----	-----	1.2196	5
322	-----	-----	1.1793	5
306	-----	-----	1.1653	6
1·0·10	-----	-----	1.1379	4
219	-----	-----	1.0855	3
228	-----	-----	1.0622	5
2·0·10	-----	-----	1.0358	4
326	-----	-----	1.0263	7
332	-----	-----	1.0072	4
2·1·10	-----	-----	0.9661	4
334	-----	-----	.9355	4
1·1·12	-----	-----	.9287	3
416	-----	-----	.9114	3
407	-----	-----		

Pattern	1	2	3
Hanawalt, Rinn, and Frevel.	102	114	212
National Bureau of Standards.	102	114	212

Structural data. Balconi [2] in 1948 determined that zinc iodide has mercuric iodide-type structure, the space group P4₁/nmc (No. 137), and (ZnI₂) per unit cell.

Two other forms of zinc iodide have been reported in the literature. One form has the cadmium iodide-type structure, according to Yamaguchi [3]; the other has cadmium chloride-type structure, according to Pinsker, Tatarinova, and Novikova [4].

The unit-cell measurements reported by Balconi are compared with the NBS lattice constants.

Lattice constants

		<i>a</i>	<i>c</i>
		<i>A</i>	<i>A</i>
1948	Balconi.	4.27	11.80
1959	National Bureau of Standards.	4.338	11.788 at 25° C

The density of zinc iodide calculated from the NBS lattice constants is 4.777 g/cm³ at 25° C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10**, 457-512 (1938).
- [2] M. Balconi, La struttura dello ZnI₂, Rend. soc. mineralog. ital. **5**, 46-51 (1948).
- [3] S. Yamaguchi, Determining the crystal structure of hygroscopic substances by electron diffraction, Sci. Papers Inst. Phys. Chem. Research (Tokyo) **39**, 357-359 (1942).
- [4] Z. G. Pinsker, L. I. Tatarinova, and V. A. Novikova, Electronographic determination of the structure of zinc iodide, Zhur. Fiz. Khim. SSSR **20**, 1401-1402 (1946)

CUMULATIVE INDEX TO VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, AND 9*

	Volume	Page		Volume	Page
Aluminum, Al	1	11	Beryllium aluminum silicate (beryl)		
Aluminum antimony, AlSb	4	72	Be ₂ Al ₂ (SiO ₃) ₆	9	13
Aluminum calcium sulfate hydrate (ettringite), Al ₂ O ₃ ·6CaO·3SO ₃ ·3H ₂ O	8	3	Beryllium orthosilicate (phenacite), Be ₂ SiO ₄	8	11
Aluminum chloride hexahydrate (chloraluminumite), AlCl ₃ ·6H ₂ O	7	3	Beryllium oxide (bromellite), BeO	3	36
Aluminum oxide, alpha (corundum), α-Al ₂ O ₃	9	3	Bismuth, Bi	3	20
Aluminum oxide monohydrate, alpha (böhmite), Al ₂ O ₃ ·H ₂ O	3	38	Bismuth (III) iodide, BiI ₃	6	20
Aluminum oxide monohydrate, beta (diaspore), Al ₂ O ₃ ·H ₂ O	3	41	Bismuth oxybromide, BiOBr	8	14
Ammonium aluminum sulfate dodecahydrate, NH ₄ Al(SO ₄) ₂ ·12H ₂ O	6	3	Bismuth oxychloride (bismoclite), BiOCl	4	54
Ammonium azide, NH ₄ N ₃	9	4	Bismuth oxyiodide, BiOI	9	16
Ammonium bicarbonate (teschemacherite), (NH ₄)HCO ₃	9	5	Bismuth sulfide (bismuthinite), Bi ₂ S ₃	4	23
Ammonium bromide, NH ₄ Br	2	49	Cadmium, Cd	3	10
Ammonium bromosmate, (NH ₄) ₂ OsBr ₆	3	71	Cadmium bromide, CdBr ₂	9	17
Ammonium bromoplatinate, (NH ₄) ₂ PtBr ₆	9	6	Cadmium carbonate (otavite), CdCO ₃	7	11
Ammonium bromoselenate, (NH ₄) ₂ SeBr ₆	8	4	Cadmium chloride, CdCl ₂	9	18
Ammonium bromotellurate, (NH ₄) ₂ TeBr ₆	8	5	Cadmium molybdate, CdMoO ₄	6	21
Ammonium chloride (sal-ammoniac), NH ₄ Cl	1	59	Cadmium oxide, CdO	2	27
Ammonium chloroiridate, (NH ₄) ₂ IrCl ₆	8	6	Cadmium selenide, CdSe, (hexagonal)	7	12
Ammonium chloropalladate, (NH ₄) ₂ PdCl ₆	8	7	Cadmium sulfide (greenockite), CdS	4	15
Ammonium chloropalladite, (NH ₄) ₂ PdCl ₄	6	6	tri-Calcium aluminate, 3CaO·Al ₂ O ₃	5	10
Ammonium chloroplatinate, (NH ₄) ₂ PtCl ₆	5	3	Calcium aluminate 12:7, 12CaO·7Al ₂ O ₃	9	20
Ammonium chlorostannate (NH ₄) ₂ SnCl ₆	5	4	Calcium bromide hexahydrate, CaBr ₂ ·6H ₂ O	8	15
Ammonium chlortellurate, (NH ₄) ₂ TeCl ₆	8	8	Calcium carbonate (aragonite), CaCO ₃	3	53
Ammonium chromium sulfate dodecahydrate, NH ₄ Cr(SO ₄) ₂ ·12H ₂ O	6	7	Calcium carbonate (calcite) CaCO ₃	2	51
Ammonium dihydrogen phosphate, NH ₄ H ₂ PO ₄	4	64	Calcium chromate, CaCrO ₄	7	13
Ammonium fluogermanate, (NH ₄) ₂ GeF ₆	6	8	Calcium fluoride (fluorite), CaF ₂	1	69
Ammonium fluosilicate (cryptohalite), (NH ₄) ₂ SiF ₆	5	5	Calcium formate, Ca(HCO ₂) ₂	8	16
Ammonium gallium sulfate dodecahydrate, NH ₄ Ga(SO ₄) ₂ ·12H ₂ O	6	9	Calcium hydroxide (portlandite), Ca(OH) ₂	1	58
Ammonium iodide, NH ₄ I	4	56	Calcium iron silicate (andradite), Ca ₃ Fe ₂ Si ₃ O ₁₂	9	22
Ammonium iron sulfate dodecahydrate, NH ₄ Fe(SO ₄) ₂ ·12H ₂ O	6	10	Calcium molybdate (powellite), CaMoO ₄	6	22
Ammonium metavanadate, NH ₄ VO ₃	8	9	Calcium nitrate, Ca(NO ₃) ₂	7	14
Ammonium nitrate (ammonia-niter), NH ₄ NO ₃	7	4	Calcium oxide, CaO	1	43
Ammonium oxalate monohydrate (oxammite), (NH ₄) ₂ C ₂ O ₄ ·H ₂ O	7	5	Calcium sulfate (anhydrite), CaSO ₄	4	65
Ammonium perchlorate, NH ₄ ClO ₄ , (orthorhombic)	7	6	Calcium sulfide (oldhamite), CaS	7	15
Ammonium perrrhenate, NH ₄ ReO ₄	9	7	Calcium tungstate (scheelite), CaWO ₄	6	23
Ammonium phosphomolybdate tetrahydrate, (NH ₄) ₃ PO ₄ (MoO ₃) ₁₂ ·4H ₂ O	8	10	Carbon (diamond), C	2	5
Ammonium sulfate (mascagnite), (NH ₄) ₂ SO ₄	9	8	Cerium(III) fluoride, CeF ₃	8	17
Ammonium zirconium fluoride (NH ₄) ₃ ZrF ₇	6	14	Cerium(IV) oxide (cerianite) CeO ₂	1	56
Antimony, Sb	3	14	Cesium aluminum sulfate dodecahydrate, CsAl(SO ₄) ₂ ·12H ₂ O	6	25
Antimony (III) iodide, SbI ₃	6	16	Cesium bromate, CsBrO ₃	8	18
Antimony (III) sulfide (stibnite), Sb ₂ S ₃	5	6	Cesium bromide, CsBr	3	49
Antimony trioxide (senarmonite), Sb ₂ O ₃	3	31	Cesium bromoplatinate, Cs ₂ PtBr ₆	8	19
Arsenic, As	3	6	Cesium bromoselenate, Cs ₂ SeBr ₆	8	20
Arsenic (III) iodide, AsI ₃	6	17	Cesium bromotellurate, Cs ₂ TeBr ₆	9	24
Arsenic trioxide (arsenolite), As ₂ O ₃	1	51	Cesium chlorate, CsClO ₃	8	20
Barium, Ba	4	7	Cesium chloride, CsCl	2	44
Barium carbonate (witherite), BaCO ₃	2	54	Cesium chloroplatinate, Cs ₂ PtCl ₆	5	14
Barium fluoride, BaF ₂	1	70	Cesium chlorostannate, Cs ₂ SnCl ₆	5	16
Barium molybdate, BaMoO ₄	7	7	Cesium chromium sulfate dodecahydrate, CsCr(SO ₄) ₂ ·12H ₂ O	8	21
Barium nitrate (nitrobarite), Ba(NO ₃) ₂	1	81	Cesium dichloriodide, CsICl ₂	3	50
Barium peroxide, BaO ₂	6	18	Cesium fluoroborate, CsBF ₄	8	22
Barium sulfate (barite), BaSO ₄	3	65	Cesium fluogermanate, Cs ₂ GeF ₆	5	17
Barium sulfide, BaS	7	8	Cesium fluoplatinate, Cs ₂ PtF ₆	6	27
Barium titanate, BaTiO ₃	3	45	Cesium fluosilicate, Cs ₂ SiF ₆	5	19
Barium tungstate, BaWO ₄	7	9	Cesium gallium sulfate dodecahydrate, CsGa(SO ₄) ₂ ·12H ₂ O	8	23
Barium zirconate, BaZrO ₃	5	8	Cesium iodide, CsI	4	47
Beryllium aluminum oxide (chrysoberyl), BeAl ₂ O ₄	9	10	Cesium iron sulfate dodecahydrate, CsFe(SO ₄) ₂ ·12H ₂ O	6	28
			Cesium nitrate, CsNO ₃	9	25
			Cesium sulfate, Cs ₂ SO ₄	7	17
			Chromium, Cr	5	20
			Chromium orthophosphate, beta, β-CrPO ₄	9	26
			Chromium (III) oxide, Cr ₂ O ₃	5	22
			Chromium silicide, Cr ₃ Si	6	29
			Cobalt aluminum oxide, CoAl ₂ O ₄	9	27
			Cobalt (II) oxide, CoO	9	28
			Cobalt (II, III) oxide, Co ₃ O ₄	9	29
			Copper, Cu	1	10
			Copper(I) bromide, CuBr	4	36
			Copper(I) chloride (nantokite), CuCl	4	35
			Copper(I) iodide (marshite), CuI	4	38
			Copper(I) oxide (cuprite), Cu ₂ O	2	23
			Copper(II) oxide (tenorite), CuO	1	49

* Further work on this program is in progress, and it is anticipated that additional volumes will be issued. Therefore, the accumulative index here is not necessarily the concluding index for the project.

	Volume	Page		Volume	Page
Copper(II) sulfide (covellite), CuS	4	13	Mercury(I) bromide, Hg ₂ Br ₂	7	33
Dysprosium sesquioxide, Dy ₂ O ₃	9	30	Mercury(I) chloride (calomel), Hg ₂ Cl ₂	1	72
Erbium phosphate, ErPO ₄	9	31	Mercury(II) chloride, HgCl ₂	1	73
Erbium sesquioxide, Er ₂ O ₃	8	25	Mercury(II) cyanide, Hg(CN) ₂	6	35
Gallium, Ga	2	9	Mercury(I) iodide, HgI	4	49
Gallium antimonide, GaSb	6	30	Mercury(II) iodide, HgI ₂	1	74
Gallium oxide, alpha, Ga ₂ O ₃	4	25	Mercury(II) oxide (montroydite), HgO (revised)	9	39
Gallium phosphate, (α-quartz type) GaPO ₄	8	27	Mercury(II) selenide (tiemannite), HgSe	7	35
Germanium, Ge	1	18	Mercury(II) sulfide (cinnabar), HgS (hexagonal)	4	17
Germanium dioxide, GeO ₂	8	28	Mercury(II) sulfide (metacinnabar), HgS (cubic)	4	21
Germanium (IV) iodide, GeI ₄	5	25	Molybdenum, Mo	1	20
Germanium oxide, GeO ₂	1	51	Molybdenum disulfide (molybdenite), MoS ₂	5	47
Gold, Au	1	33	Molybdenum trioxide (molybdate), MoO ₃	3	30
Gold antimony 1:2 (aurostibite), AuSb ₂	7	18	Neodymium ethylsulfate nonahydrate, Nd[(C ₂ H ₅)SO ₄] ₃ ·9H ₂ O	9	41
Gold tin 1:1 AuSn	7	19	Neodymium fluoride, NdF ₃	8	36
Hafnium, Hf	3	18	Neodymium oxide, Nd ₂ O ₃	4	26
Holmium sesquioxide, Ho ₂ O ₃	9	32	Neodymium oxychloride, NdOCl	8	37
Indium, In	3	12	Nickel, Ni	1	13
Indium antimony, InSb	4	73	Nickel aluminate, NiAl ₂ O ₄	9	42
Indium oxide, In ₂ O ₃	5	26	Nickel fluosilicate hexahydrate, NiSiF ₆ ·6H ₂ O	8	38
Indium phosphate, InPO ₄	8	29	Nickel germanate, Ni ₂ GeO ₄	9	43
Iodic acid, HIO ₃	5	28	Nickel(II) oxide (bunsenite), NiO	1	47
Iodine, I ₂	3	16	Nickel sulfate hexahydrate, NiSO ₄ ·6H ₂ O	7	36
Iridium, Ir	4	9	Niobium silicide, NbSi ₂	8	39
Iron, alpha, Fe	4	3	Osmium, Os	4	8
Iron sulfide (pyrite), FeS ₂	5	29	Palladium, Pd	1	21
Lanthanum fluoride, LaF ₃	7	21	Palladium oxide, PdO	4	27
Lanthanum oxide, La ₂ O ₃	3	33	Platinum, Pt	1	31
Lanthanum oxychloride, LaOCl	7	22	Potassium aluminum sulfate dodecahydrate, KAl(SO ₄) ₂ ·12H ₂ O	6	36
Lead, Pb	1	34	Potassium borohydride, KBH ₄	9	44
Lead bromide, PbBr ₂	2	47	Potassium bromate, KBrO ₃	7	38
Lead carbonate (cerussite), PbCO ₃	2	56	Potassium bromide, KBr	1	66
Lead chloride (cotunnite), PbCl ₂	2	45	Potassium bromoplatinate, K ₂ PtBr ₆	8	40
Lead formate, Pb(HCO ₂) ₂	8	30	Potassium bromoselenate, K ₂ SeBr ₆	8	41
Lead fluochloride (matlockite) PbFCl	1	76	Potassium chloride (sylvite), KCl	1	65
Lead fluoride, alpha, PbF ₂	5	31	Potassium chloroplatinate, K ₂ PtCl ₆	5	49
Lead fluoride, beta, PbF ₂	5	33	Potassium chlorostannate K ₂ SnCl ₆	6	38
Lead(II) iodide, PbI ₂	5	34	Potassium chromium sulfate dodecahydrate, KCr(SO ₄) ₂ ·12H ₂ O	6	39
Lead molybdate (wulfenite), PbMoO ₄	7	23	Potassium cobaltinitrite, K ₃ Co(NO ₂) ₆	9	45
Lead monoxide (litharge), PbO (red)	2	30	Potassium cyanate, KCNO	7	39
Lead monoxide (massicot) PbO (yellow)	2	32	Potassium cyanide, KCN	1	77
Lead nitrate, Pb(NO ₃) ₂	5	36	Potassium dihydrogen phosphate, KH ₂ PO ₄	3	69
Lead(II, III) oxide (minimum), Pb ₃ O ₄	8	32	Potassium fluogermanate, K ₂ GeF ₆	6	41
Lead, phosphate hydrate (lead hydroxyapatite), Pb ₅ (PO ₄) ₃ OH	8	33	Potassium fluoplatinate, K ₂ PtF ₆	6	42
Lead selenide (clausthalite), PbSe	5	38	Potassium fluoride, KF	1	64
Lead sulfate (anglesite), PbSO ₄	3	67	Potassium fluosilicate (hieratite), K ₂ SiF ₆	5	50
Lead sulfide (galena), PbS	2	18	Potassium fluotitanate, K ₂ TiF ₆	7	40
Lead titanate, PbTiO ₃	5	39	Potassium heptafluozirconate, K ₃ ZrF ₇	9	46
Lead tungstate (stolzite), PbWO ₄	7	24	Potassium iodide, KI	1	68
Lithium bromide, LiBr	4	30	Potassium metaperiodate, KIO ₄	7	41
Lithium chloride, LiCl	1	62	Potassium nitrate (niter), KNO ₃	3	58
Lithium fluoride, LiF	1	61	Potassium perchlorate, KClO ₄	6	43
Lithium iodate, LiIO ₃	7	26	Potassium permanganate, KMnO ₄	7	42
Lithium nitrate, LiNO ₃	7	27	Potassium perhenate, KReO ₄	8	41
Lithium perchlorate trihydrate, LiClO ₄ ·3H ₂ O	8	34	Potassium phosphomolybdate, tetrahydrate, K ₃ PO ₄ (MoO ₃) ₁₂ ·4H ₂ O	8	43
Magnesium, Mg	1	10	Potassium sulfate (arcanite), K ₂ SO ₄	3	62
Magnesium aluminate (spinel), MgAl ₂ O ₄	2	35	Potassium thiocyanate, KCNS	8	44
Magnesium carbonate (magnesite), MgCO ₃	7	28	Potassium zinc fluoride, K ₂ ZnF ₆	5	51
Magnesium chromite (picrochromite), MgCr ₂ O ₄	9	34	Praseodymium fluoride, PrF ₃	5	52
Magnesium fluoride (sellaite), MgF ₂	4	33	Praseodymium oxychloride, PrOCl	9	47
Magnesium hydroxide (brucite), Mg(OH) ₂	6	30	Rhenium, Re	2	13
Magnesium oxide (periclase), MgO	1	37	Rhodium, Rh	3	9
Magnesium silicate (enstatite), MgSiO ₃	6	32	Rubidium aluminum sulfate dodecahydrate, RbAl(SO ₄) ₂ ·12H ₂ O	6	44
Magnesium silicate (forsterite), Mg ₂ SiO ₄	1	83	Rubidium bromate, RbBrO ₃	8	45
Magnesium sulfate heptahydrate (epsomite), MgSO ₄ ·7H ₂ O	7	30	Rubidium bromide, RbBr	7	43
Magnesium sulfide, MgS	7	31	Rubidium bromotellurate, Rb ₂ TeBr ₆	8	46
Magnesium tin, Mg ₂ Sn	5	41	Rubidium chlorate, RbClO ₃	8	47
Magnesium titanate (geikielite), MgTiO ₃	5	43	Rubidium chloride, RbCl	4	41
Magnesium tungstate, MgWO ₄	1	84	Rubidium chloroplatinate, Rb ₂ PtCl ₆	5	53
Manganese aluminate (galaxite), MnAl ₂ O ₄	9	35	Rubidium chlorostannate, Rb ₂ SnCl ₆	6	46
Manganese(II) carbonate (rhodochrosite), MnCO ₃	7	32	Rubidium chlorotellurate, Rb ₂ TeCl ₆	8	48
Manganese ferrite (jacobsite), MnFe ₂ O ₄	9	36			
Manganese(II) oxide (manganosite), MnO	5	45			
Manganese(III) oxide (partridgeite), Mn ₂ O ₃	9	37			
Manganese sulfide, alpha (alabandite), α-MnS	4	11			

Volume	Page	Volume	Page
Rubidium chromium sulfate dodecahydrate, $\text{RbCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6 47	Sulfur, S	9 54
Rubidium fluoplatinate, Rb_2PtF_6	6 48	Tantalum, Ta	1 29
Rubidium fluosilicate, Rb_2SiF_6	6 49	Tantalum Silicide, TaSi_2	8 59
Rubidium iodide, RbI	4 43	Tellurium, Te	1 26
Rubidium sulfate, Rb_2SO_4	8 48	Tellurium(IV) oxide (paratellurite) TeO_2 (tetragonal)	7 56
Ruthenium, Ru	4 5	Tellurium(IV) oxide (tellurite), TeO_2 (orthorhombic)	9 57
Scandium oxide, Sc_2O_3	3 27	Thallium aluminum sulfate dodecahydrate, $\text{TlAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6 53
Scandium phosphate, ScPO_4	8 50	Thallium(I) bromate, TlBrO_3	8 60
Selenium, Se	5 54	Thallium bromide, TlBr	7 57
Selenium dioxide (selenolite), SeO_2	1 53	Thallium(I) chlorate, TlClO_3	8 61
Silicon, Si	2 6	Thallium(I) chloride, TlCl	4 51
Silicon dioxide (alpha or low quartz), SiO_2	3 24	Thallium chloroplatinate, Tl_2PtCl_6	5 70
Silicon dioxide (alpha or low cristobalite), SiO_2	1 39	Thallium chlorostannate, Tl_2SnCl_6	6 54
Silicon dioxide (beta or high cristobalite), SiO_2	1 42	Thallium chromium sulfate dodecahydrate, $\text{TlCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6 55
Silver, Ag	1 23	Thallium fluosilicate, Tl_2SiF_6	6 56
Silver arsenate, Ag_3AsO_4	5 56	Thallium gallium sulfate dodecahydrate, $\text{TlGa}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6 57
Silver bromate, AgBrO_3	5 57	Thallium(I) iodate, TlIO_3	8 62
Silver bromide (bromyrite), AgBr	4 46	Thallium(I) iodide, TlI (orthorhombic)	4 53
Silver chlorate, AgClO_3	7 44	Thallium(I) nitrate, TlNO_3	6 58
Silver chloride (cerargyrite), AgCl	4 44	Thallium(III) oxide, Tl_2O_3	2 28
Silver iodide (iodyrite), AgI (hexagonal)	8 51	Thallium(I) phosphate, Tl_3PO_4	7 58
Silver iodide, gamma, $\gamma\text{-AgI}$	9 48	Thallium(III) phosphate, TlPO_4	7 59
Silver metaperiodate, AgIO_4	9 49	Thallium(I) sulfate, Tl_2SO_4	6 59
Silver molybdate, Ag_2MoO_4	7 45	Thallium(I) thiocyanate, TlCNS	8 63
Silver nitrate, AgNO_3	5 59	Thorium oxide (thorianite), ThO_2	1 57
Silver nitrite, AgNO_2	5 60	Thulium sesquioxide, Tm_2O_3	9 58
Silver(II) oxynitrate, $\text{Ag}_2\text{O}_3\text{NO}_2$	4 61	Tin, alpha, Sn	2 12
Silver perrhenate, AgReO_4	8 53	Tin, beta, Sn	1 24
Silver phosphate, Ag_3PO_4	5 62	Tin(IV) iodide, SnI_4	5 71
Silver sulfate, Ag_2SO_4	7 46	Tin(II) oxide, SnO	4 28
Sodium acid fluoride, NaHF_2	5 63	Tin(IV) oxide (cassiterite), SnO_2	1 54
Sodium borohydride, NaBH_4	9 51	Tin(II) telluride, SnTe	7 61
Sodium bromate, NaBrO_3	5 65	Titanium, Ti	3 1
Sodium bromide, NaBr	3 47	Titanium dioxide (anatase), TiO_2	1 46
Sodium carbonate monohydrate (thermonatrite), $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$	8 54	Titanium dioxide (rutile), TiO_2	1 44
Sodium chlorate, NaClO_3	3 51	Titanium(III) oxide, $\text{TiO}_{1.515}$	9 59
Sodium chloride (halite), NaCl	2 41	Titanium silicide, Ti_3Si_2	8 64
Sodium cyanide, NaCN (cubic)	1 78	Tungsten, W	1 28
Sodium cyanide, NaCN (orthorhombic)	1 79	Tungsten sulfide (tungstenite), WS_2	8 65
Sodium fluoride (villiaumite), NaF	1 63	Uranium dioxide, UO_2	2 33
Sodium iodate, NaIO_3	7 47	Urea, $\text{CO}(\text{NH}_2)_2$	7 61
Sodium iodide, NaI	4 31	Vanadium(V) oxide, V_2O_5	8 66
Sodium metaperiodate, NaIO_4	7 48	Yttrium oxide, Y_2O_3	3 28
Sodium nitrate (soda-niter), NaNO_3	6 50	Yttrium phosphate (xenotime), YPO_4	8 67
Sodium nitrite, NaNO_2	4 62	Zinc, Zn	1 16
Sodium perchlorate, NaClO_4 (orthorhombic)	7 49	Zinc aluminate (gahnite), ZnAl_2O_4	2 38
Sodium sulfate (thenardite), Na_2SO_4	2 59	Zinc borate, ZnB_2O_4	1 83
Sodium sulfite, Na_2SO_3	3 60	Zinc carbonate (smithsonite), ZnCO_3	8 69
Strontium bromide hexahydrate, $\text{SrBr}_2 \cdot 6\text{H}_2\text{O}$	4 60	Zinc cyanide, $\text{Zn}(\text{CN})_2$	5 73
Strontium carbonate (strontianite) SrCO_3	3 56	Zinc fluoride, ZnF_2	6 60
Strontium chloride, SrCl_2	4 40	Zinc fluosilicate hexahydrate, $\text{ZnSiF}_6 \cdot 6\text{H}_2\text{O}$	8 70
Strontium chloride hexahydrate, $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$	4 58	Zinc iodide, ZnI_2	9 60
Strontium fluoride, SrF_2	5 67	Zinc orthosilicate (willemite), Zn_2SiO_4	7 62
Strontium formate, $\text{Sr}(\text{CHO}_2)_2$	8 55	Zinc oxide (zincite), ZnO	2 25
Strontium formate dihydrate, $\text{Sr}(\text{CHO}_2)_2 \cdot 2\text{H}_2\text{O}$ orthorhombic	8 56	Zinc pyrosilicate hydrate (hemimorphite) $\text{Zn}_4(\text{OH})_2\text{Si}_2\text{O}_7 \cdot \text{H}_2\text{O}$	2 62
Strontium iodide hexahydrate, $\text{SrI}_2 \cdot 6\text{H}_2\text{O}$	8 58	Zinc selenide, ZnSe	3 23
Strontium molybdate, SrMoO_4	7 50	Zinc sulfate (zinkosite), ZnSO_4	7 64
Strontium nitrate, $\text{Sr}(\text{NO}_3)_2$	1 80	Zinc sulfate heptahydrate (goslarite), $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$	8 71
Strontium oxide, SrO	5 68	Zinc sulfide, alpha (wurtzite), ZnS	2 14
Strontium peroxide, SrO_2	6 52	Zinc sulfide, beta (sphalerite), ZnS	2 16
Strontium sulfate (celestite), SrSO_4	2 61	Zirconium, alpha, Zr	2 11
Strontium sulfide, SrS	7 52	Zirconium silicate (zircon), ZrSiO_4	4 68
Strontium titanate, SrTiO_3	3 44	Zirconium sulfate tetrahydrate, $\text{Zr}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$	7 66
Strontium tungstate, SrWO_4	7 53		
Strontium zirconate, SrZrO_3	9 51		
Sulfamic acid, NH_2SO_3	7 54		

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